NGT Technical Meeting
WP 1.5 - LQFT

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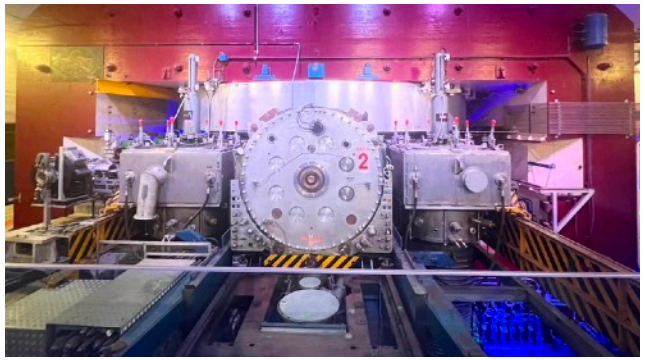
Outline

NGT WP 1
Task 1.5 (b) Lattice Quantum Field Theory

- Motivation
- Status of on-going work
  - Benchmarks and systems
- Outlook



Task 1.5: New computing strategies for data modeling and interpretation - LQFT part

Code modernization on parallel architectures and utilising AI is aligned with WP2 and WP3

- Development of software and algorithms for efficiently exploiting next-gen computer architectures use in LQFT simulations on extreme-scaling low-latency/high-bandwidth accelerator-based clusters

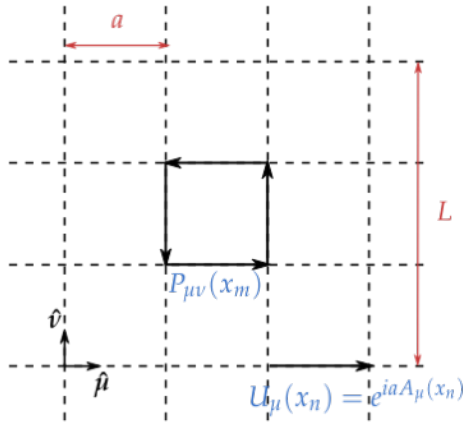
Lattice QCD:

- Nonperturbative contribution to precision physics, e.g. alpha_s, g-2, B-physics, ..

$$\langle 0|O|0\rangle = \frac{1}{Z}\int D[U,\psi,\bar{\psi}]\, O \cdot e^{-S_{lat}[U,\psi,\bar{\psi}]}$$

- Discrete 4D space time
- Ideally suited for extreme-parallelism

Degree of freedom:
SU(3) gauge links



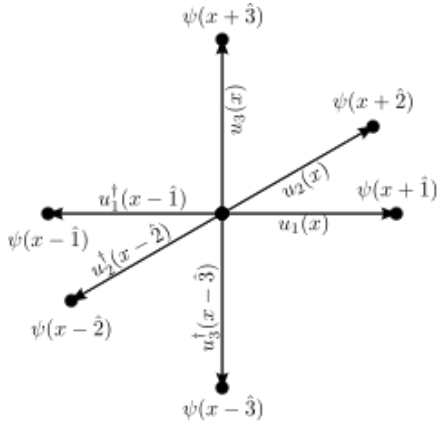
4 x L*L*L*T links with L = 96 typically

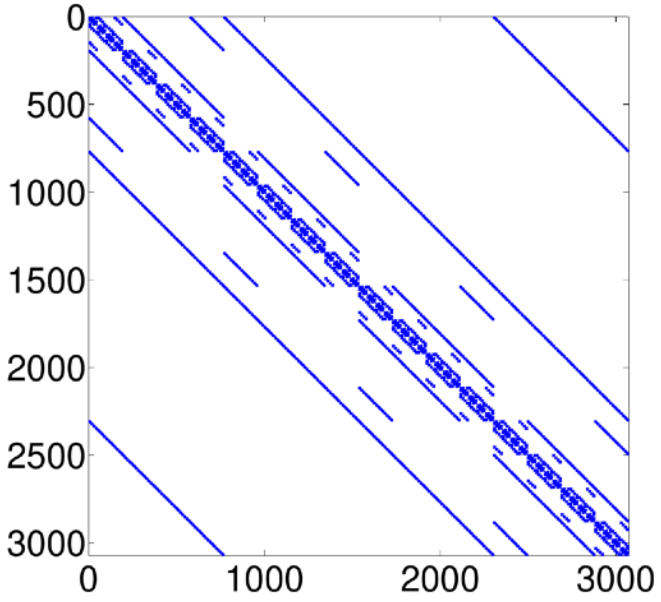
Task 1.5: HPC in LQFT

Lattice QCD:
Two core computational steps:

- Generation of field configuration (Markov chain Monte Carlo) via Molecular Dynamics
- Computation of quark propagators (Krylov-subspace solvers)

Main computational kernel:
Solve: M * x = b
with M a 4D stencil operator



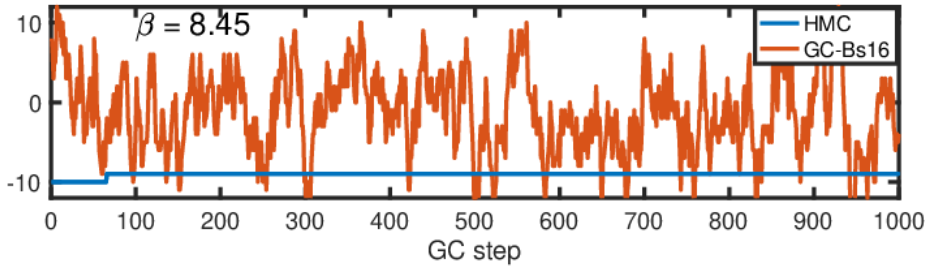


High precision requires
100+ Mi inversions

Tasks and deliverables of 2024

Milestones (M12)

- Provide benchmarking support with lattice QFT codes guiding hardware procurement and commissioning for HPC hardware.



Deliverables (M12):

Develop LQFT benchmarking software tailored to hardware infrastructure procured under 1.1.

- *Preliminary numbers from A100 and H100 collected*

Organization of several community Workshops

- *First workshop "NGT - Algorithms for lattice QCD" scheduled for 9-11 December*

Share expertise on parallelism and accelerator-based algorithms with TH/IT/CMS/ATLAS

Benchmarks with lattice QFT codes

Case selection:

Conjugate Gradient solver and multi-grid solver based on **QUDA** and **grid** (which comes also with ARM optimization)

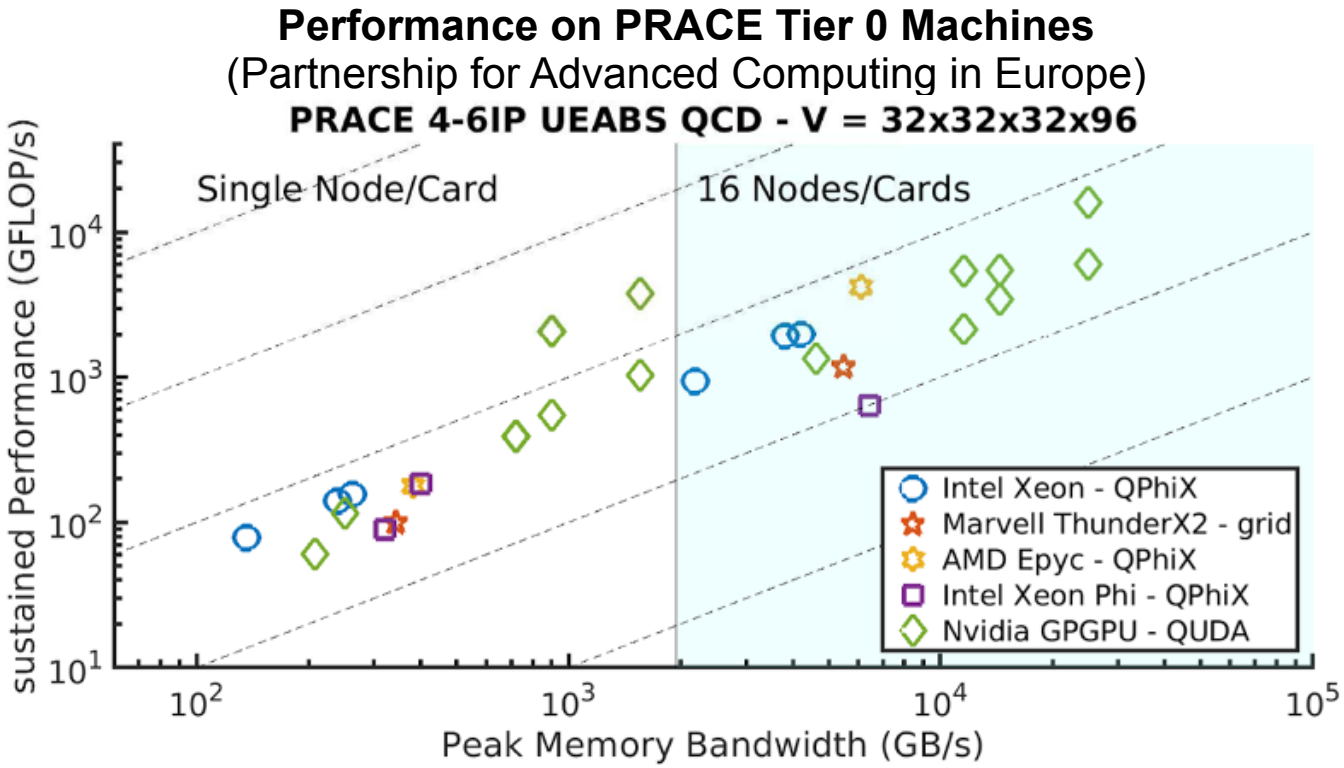
Idea: based on previous benchmark cases
- match them to newest standard

Example: UEABS under Prace
Conjugate gradient benchmark case:

$$D(U) \cdot x$$

- arithmetic intensity ~ 1.0
- computational costs grows with **V**

on HPC-hardware:
- bandwidth bound
- latency bound

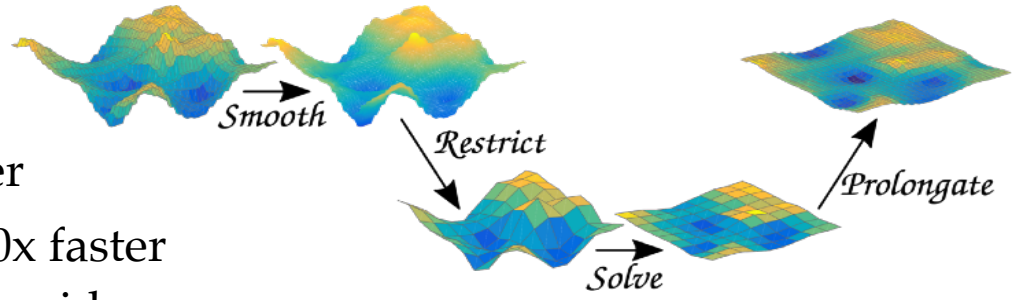


Benchmarks with lattice QFT codes

Two cases:

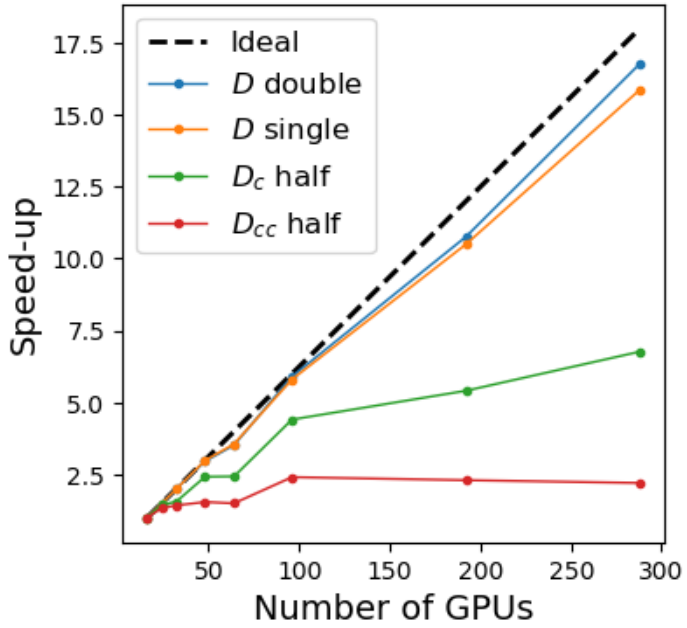
CG: Conjugate Gradient solver (traditional)

- main kernel: Dslash
- different sizes with L=32, 64, 96
- bandwidth bound: 1:1 Flop to bytes



MG: Multigrid solver

- state-of-the-art: 100x faster
- limited by coarsest grid



Access to large computing facilities

Towards Exascale computing:

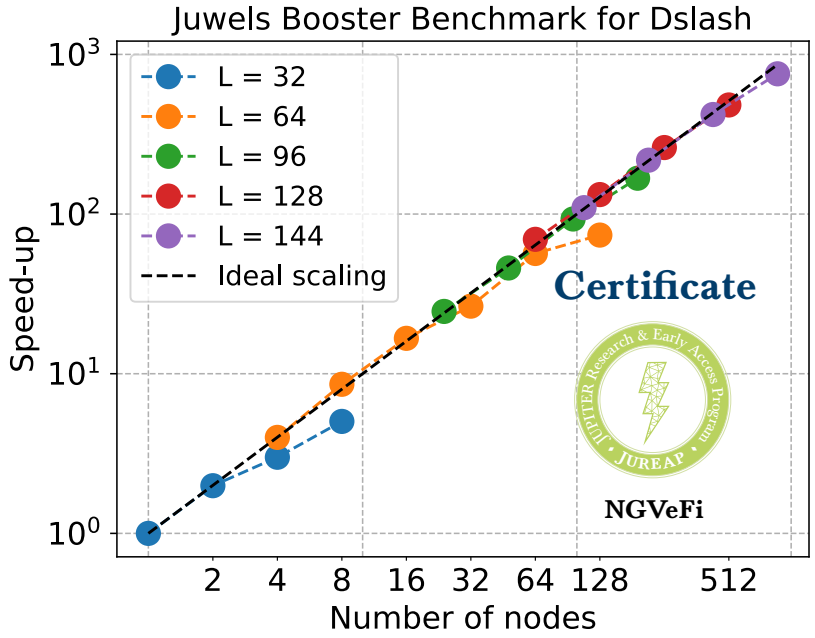
Jupiter (JSC) will be Europes first Exascale system
with 6000 Nodes each with:
- 4x Nvidia Grace Hopper chips
- connected via Infiniband NDR with 4xHCA 200 Gbit/s
Successful participation in Jureap Phase

Access to large scale systems

First large scale Grace Hopper system online
with ALPS at CSCS
- PACS software project *Alpenglue* with Bern (PI)
- supported by CSCS software engineers
- will give access to CSCS Prototype systems

CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ALPS



Utilising computational resources
to push precision physics from the lattice

- First European machine by 2025 Q1
- 8.7 Pflops on 3456 A100

NGT Algorithm workshop - Lattice QCD

Organization of Workshop: Algorithm in LQCD

- *9th - 11th December by inviting 16 speakers with Lattice QCD background*

Topics:

- *Variance reduction, novel update for MCMC simulations and adaption to novel hardware*

Mostly addressing members of the LQFT community

- *Third day will be on optimising for novel hardware (might be of interest to other NGT members/tasks)*

Indico page: https://indico.cern.ch/e/NGT_algorithms_for_latticeQCD_Dec24

Will take place in the 4-3 6 Main TH auditorium

Task 1.5: Challenges in LQFT

Workshop will address main algorithmic challenges in LQCD:

Day 1: Signal to noise problem

• high precision in baryon physics out of reach

Input for required software developments
(higher precision via localization)

Day 2: Continuum limit controlling via finer lattices

• overcoming critical slowing down via generate models

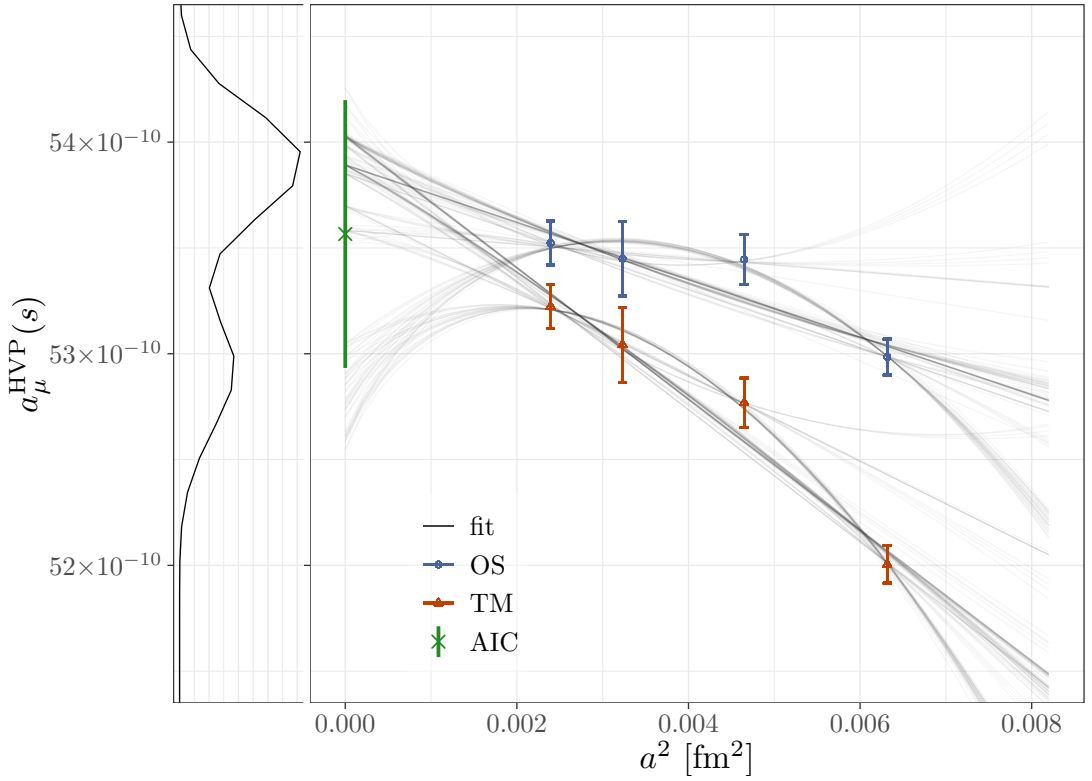
Overview on disruptive solutions, e.g. ML and traditional

Day 3: Utilization of large scale machines

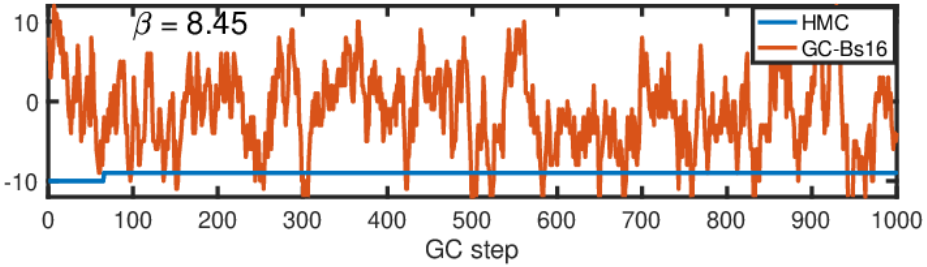
• larger lattices requires:

  • quadruple precision and strong scalability

Main developers of both state-of-the-art package will come
(Included in the benchmark cases)



Outlook to 2025



Milestones (M24)

- Port code and optimize LQFT simulation performance for new hardware that is being procured
  - *utilizing the input of the NGT algorithm workshop for LQCD*

Deliverables (M24):

Sign-off of new HPC cluster assuming new hardware performing to specs
- *using the defined benchmark kernels*

Show optimised parallel scaling performance of LQFT codes on new hardware
- by *identify scalable algorithmic solutions for LQCD challenges*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