lattice QCD software development for heterogeneous supercomputers

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Bálint Joó (Oak Ridge National Laboratory)
Dean Howarth (California Institute of Technology)
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Damian Alvarez, Ahmed Fahmy, Andreas Herten (Juelich Supercomputing Center)

deRSE24
Würzburg, Germany

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  - Describe science and how this motivates investment in the underlying research software.
  - HPC aspects of lattice field theory research.
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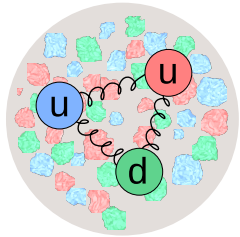
- This looks very much like many open source projects.
- Unexpected and interesting things happen as a result.

What is Lattice QCD?

The Strong Nuclear Force

- **Question: Where does the mass of a proton, m_P, come from?**



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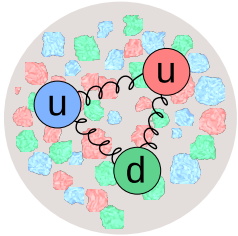

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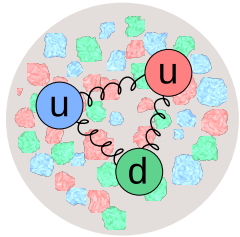

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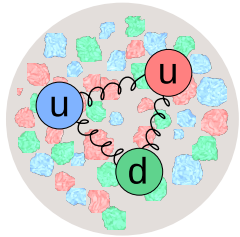

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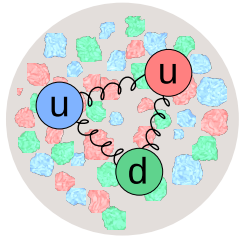

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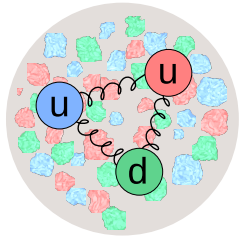

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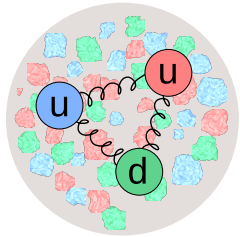

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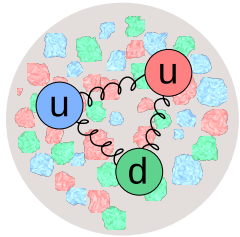

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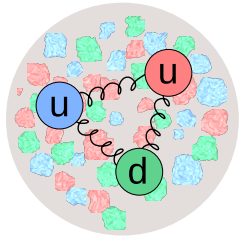

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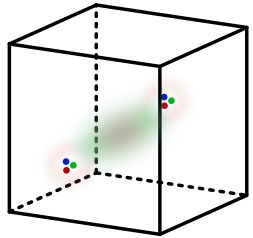

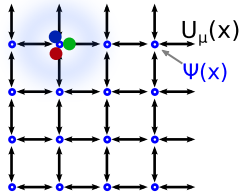

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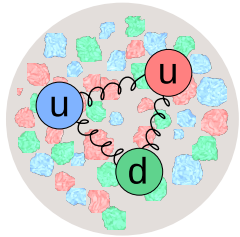

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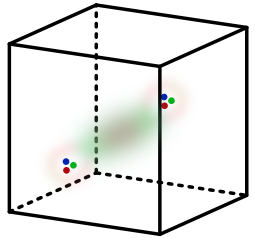

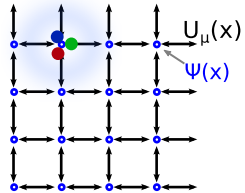

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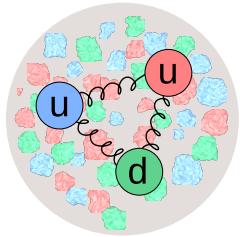

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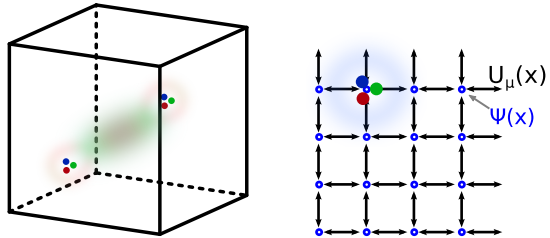

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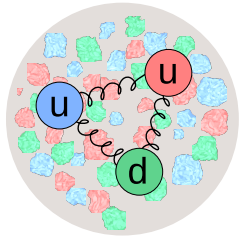

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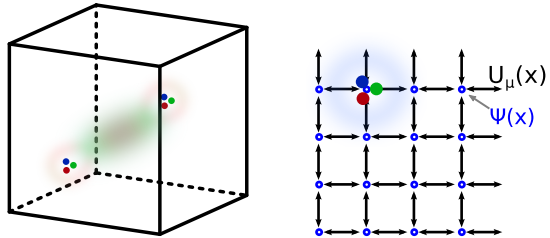

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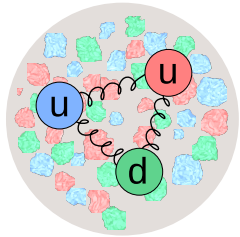

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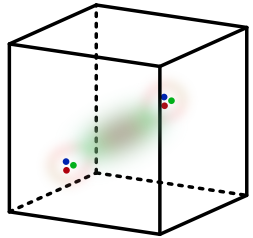

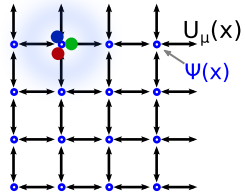

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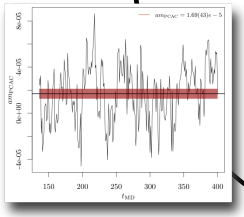
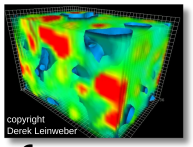
Turns out to be a numerical grand challenge!

Numerical Grand Challenge Problem

C A P A B I L I T Y

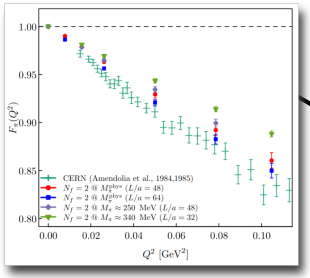
"sample vacuum"
generate ensemble





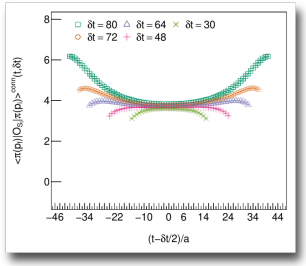
$Z = \int dU \exp(-S_{eff}[U])$

A N A L Y S I S

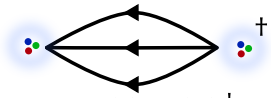


extract physical
observables

compute correlations



"excite vacuum"



$\langle \Omega \mid N(t)N(0)^\dagger \mid \Omega \rangle$

$S_q(x\text{-}y) \cong D[U]^{-1}(x,y)\psi(y)$

compute
quark propagators

C A P A C I T Y

Numerical Grand Challenge Problem

CAPABILITY

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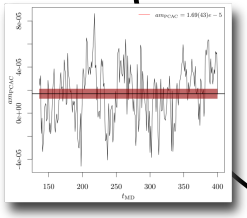

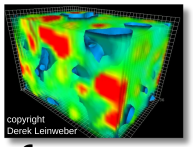

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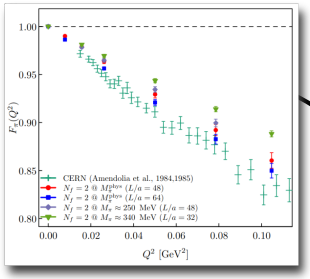
ANALYSIS



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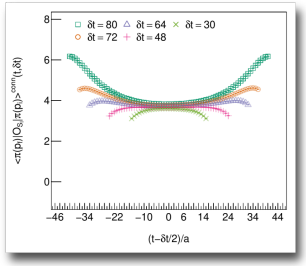

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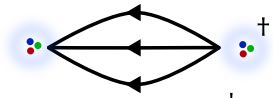

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In this talk concentrate on software for first and second stages.

The first two stages of Lattice QCD Calculations

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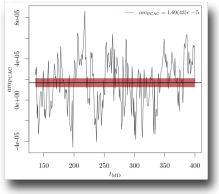
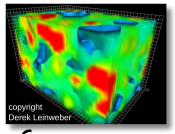




$Z = \int dU \exp(-S_{eff}[U])$

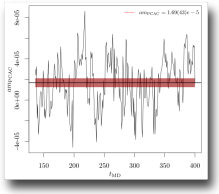
Ensemble Generation

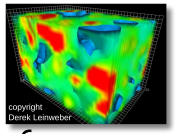
- Markov Chain Monte Carlo run on largest supercomputers in the world

The first two stages of Lattice QCD Calculations

C A P A B I L I T Y

"sample vacuum"
generate ensemble





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The first two stages of Lattice QCD Calculations

CAPABILITY

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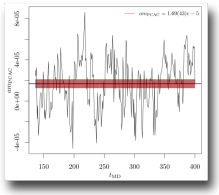

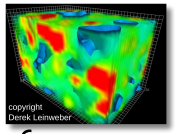

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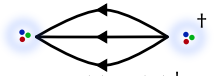
- Physics contained in correlation functions.
  - Mathematical objects which quantify interactions between different particles *created* and *annihilated* at different times

$S_q(x\text{-}y) \cong D[U]^{-1}(x,y)\psi(y)$

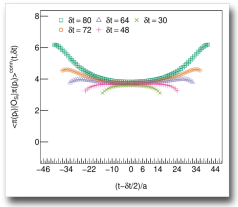
compute
quark propagators

"excite vacuum"



$\langle \Omega \mid N(t)N(0)^{\dagger} \mid \Omega \rangle$

compute correlations



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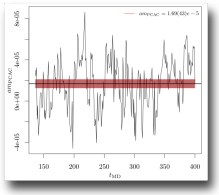

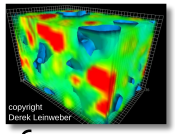

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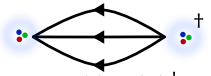

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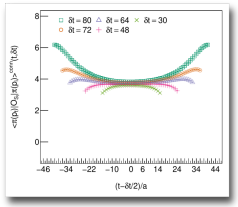

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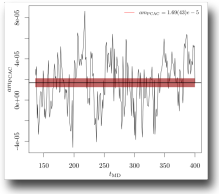

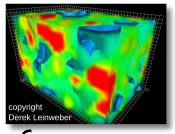

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- **Petabytes of long-term storage.**

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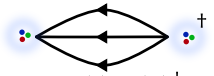

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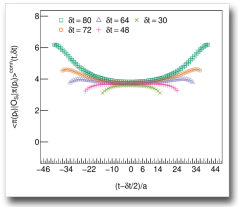

C A P A C I T Y

The Lattice Field Theory / Lattice QCD Community

- Theoretical physicists, related to high energy, particle and hadron/nuclear physics.
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  - Keep production stack running.
  - Integrate short-term postdocs and PhD students.
  - Do continuous integration on GPU hardware:
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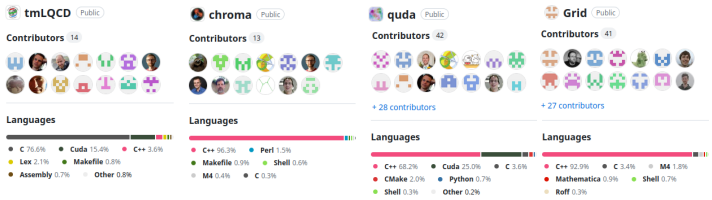
Examples of LQCD Codes and Libraries



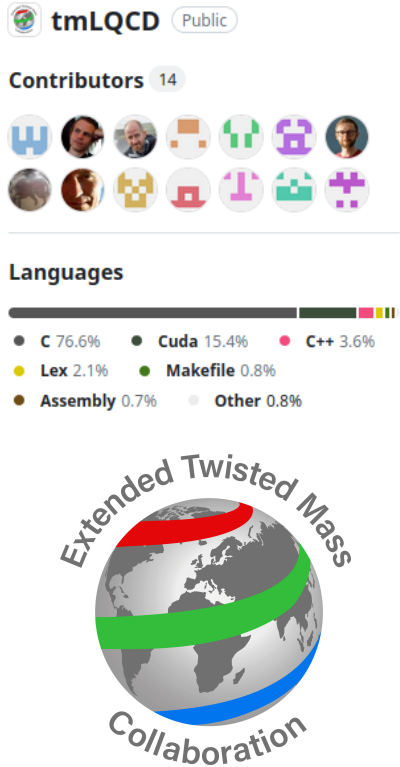
This talk: tmLQCD & QUDA

tmLQCD

Workhorse of the ETM collaboration

Software suite with 20 year history started by Carsten Urbach $\sim$ 140k LOC (C, C++).

gh.com/etmc/tmLQCD



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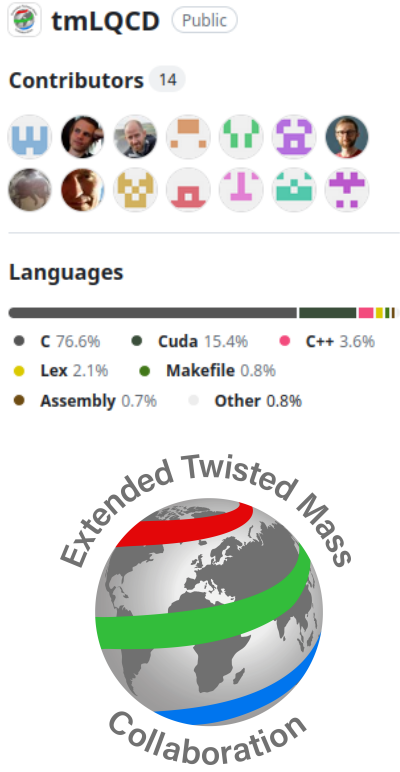

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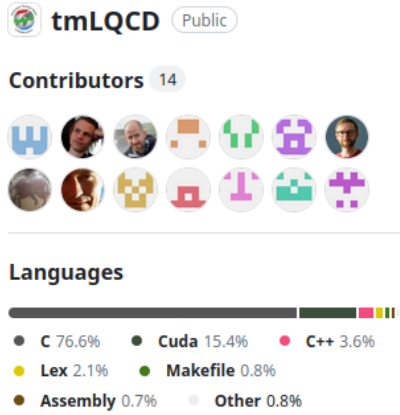

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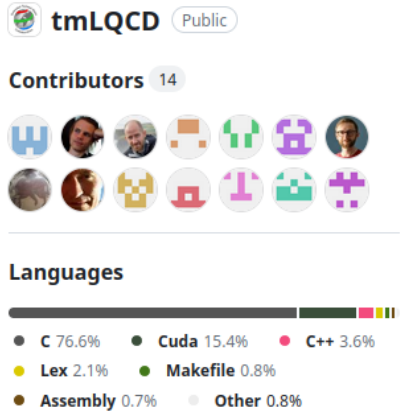

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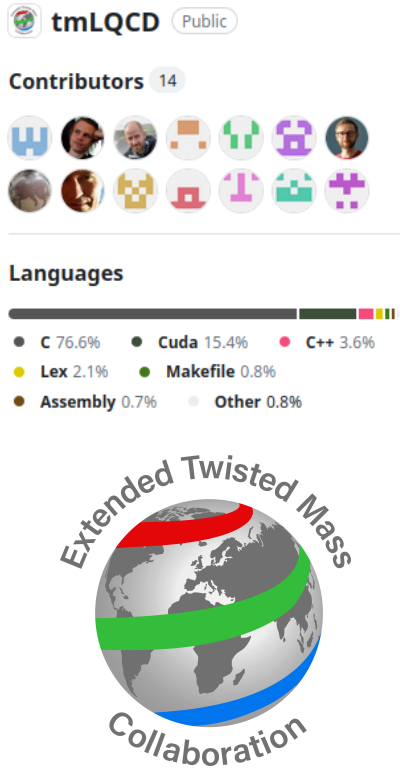

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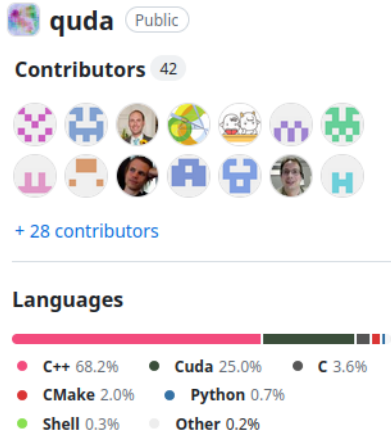

Important technical features

- Provides solvers for most fermionic discretisations & gauge evolution algorithms.
- Mixed-precision methods & autotuning of kernel launch parameters and communication policies.
- Highly efficient multigrid solver for problems with large condition number.
- NVSHMEM for improved strong scaling.
- Major performance-portability effort: HIP (merged), SYCL (in review), OpenMP (in development)

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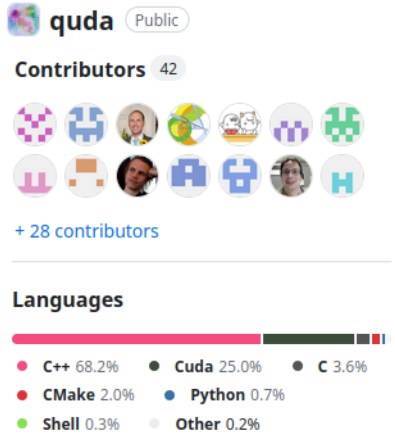

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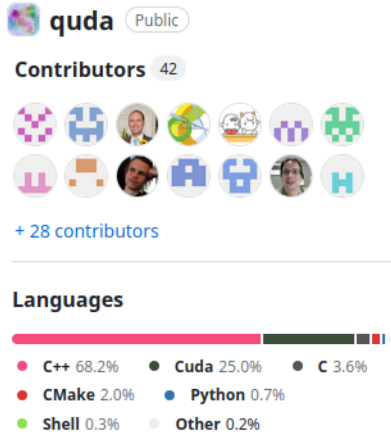

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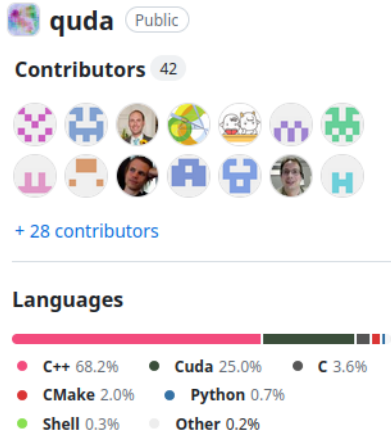

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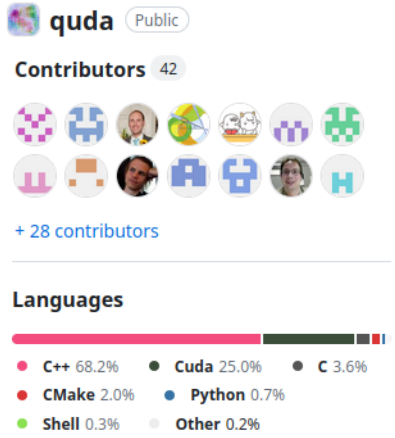
gh.com/lattice/quda



Important technical features

- Provides solvers for most fermionic discretisations & gauge evolution algorithms.
- Mixed-precision methods & autotuning of kernel launch parameters and communication policies.
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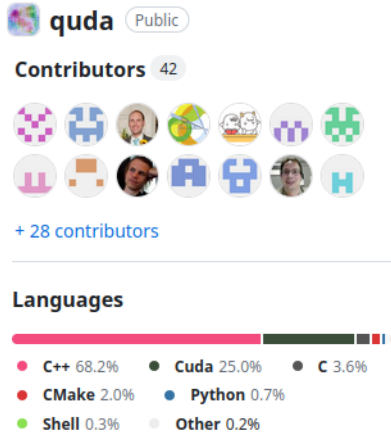

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The QUDA library and the interactions with its developers have been *essential* for us over the past years.

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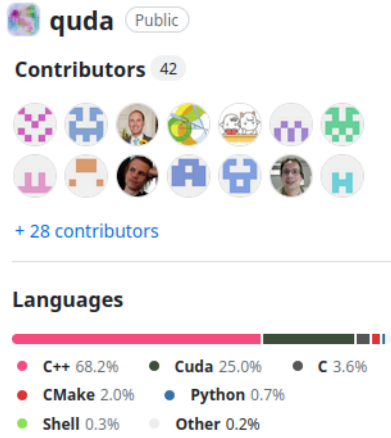

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Collaboration between Researchers, Computing Centers and Hardware Vendors

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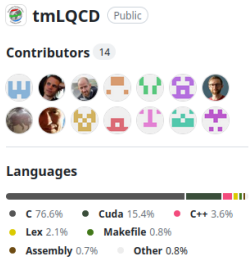
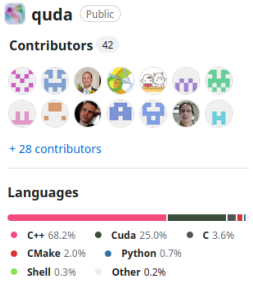


COMPUTING CENTERS



VENDORS

Working on the QUDA library

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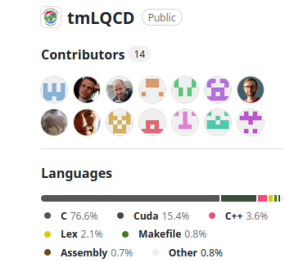

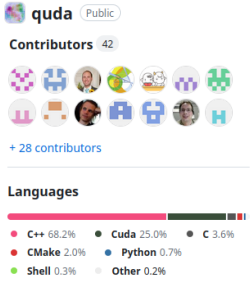

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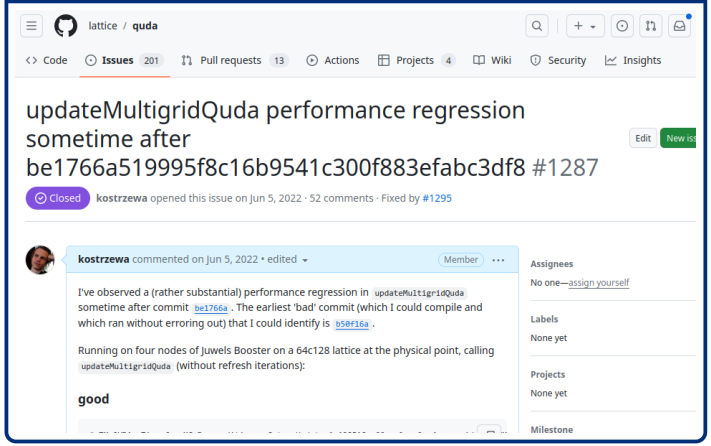

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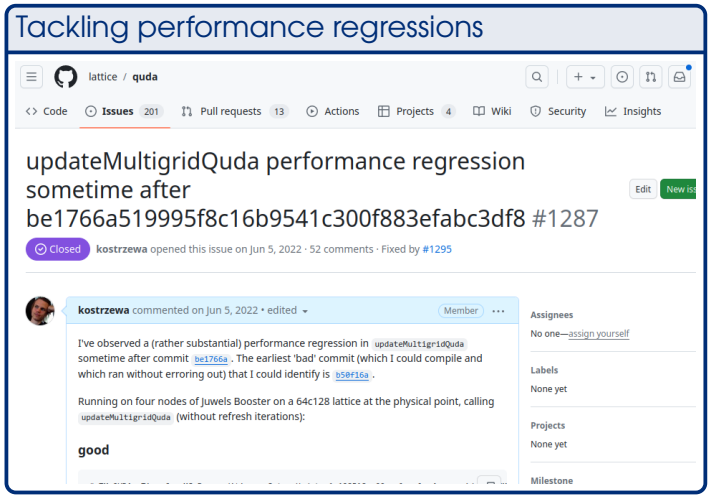

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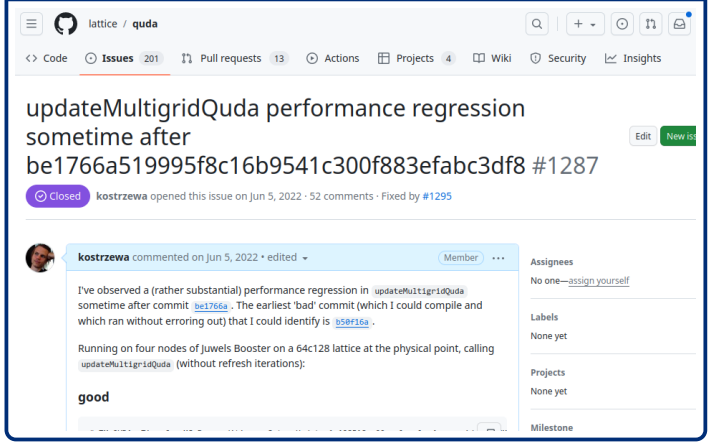
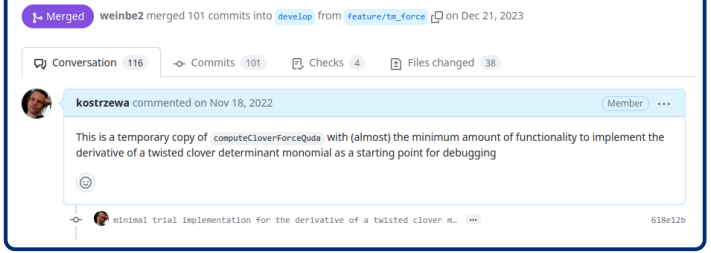


Resolution

Introduction of new features



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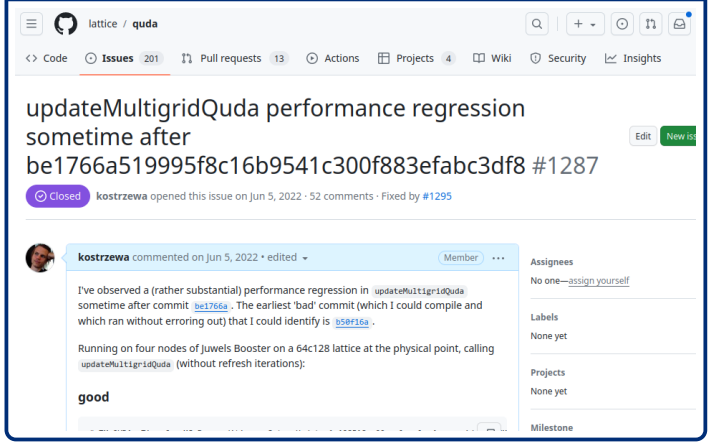

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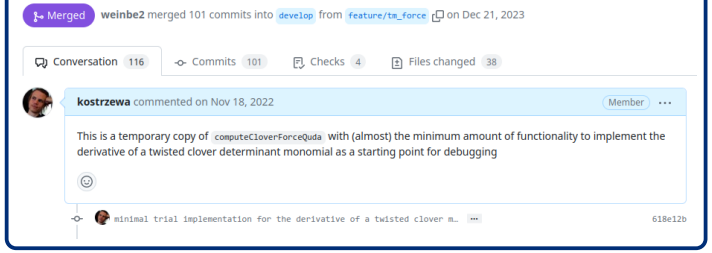
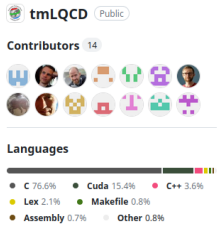


Polishing and Merging

Interaction with Juelich Supercomputing Centre (JSC)

RESEARCHERS



COMPUTING CENTERS

- JUWELS Booster Early Access Programme
- Long-term support with a very interesting issue

JUWELS Booster early access programme

Early Access to JUWELS Booster

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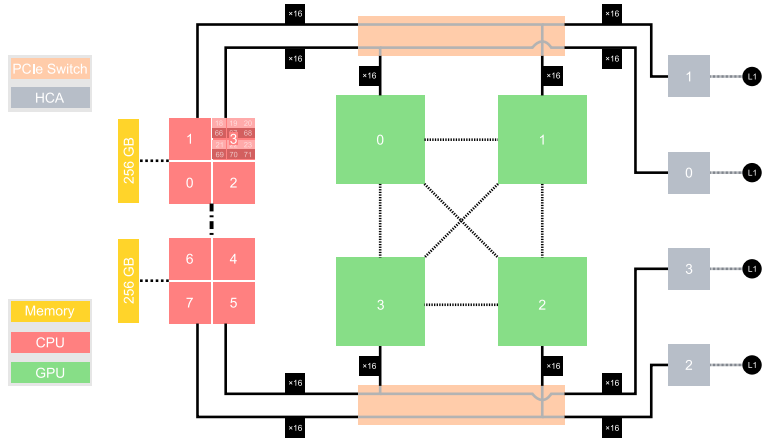

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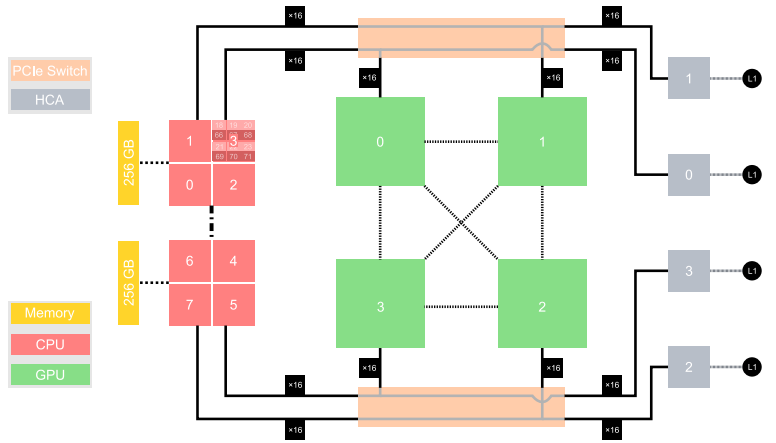

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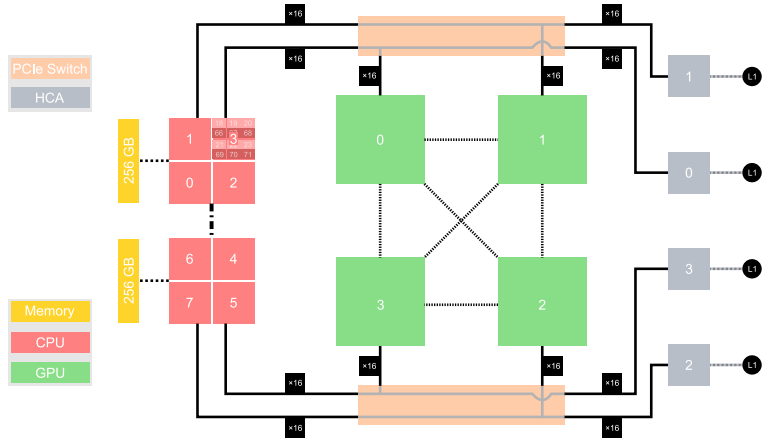

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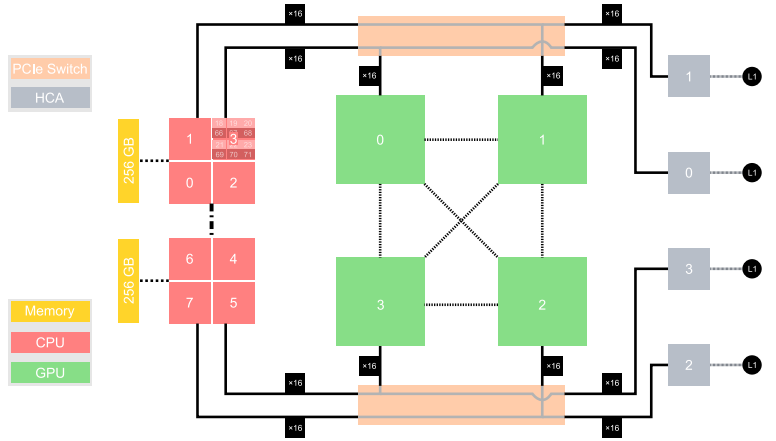

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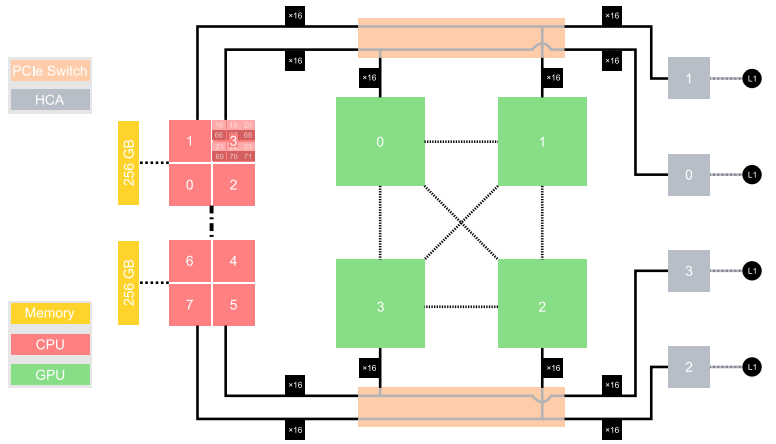

EA programme enabled many publications:

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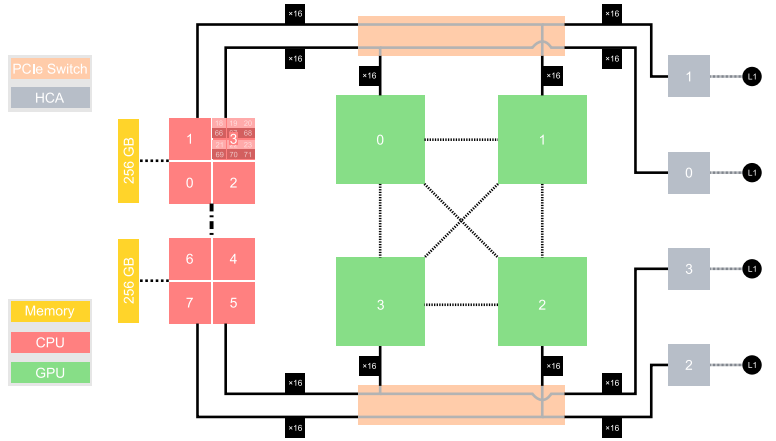

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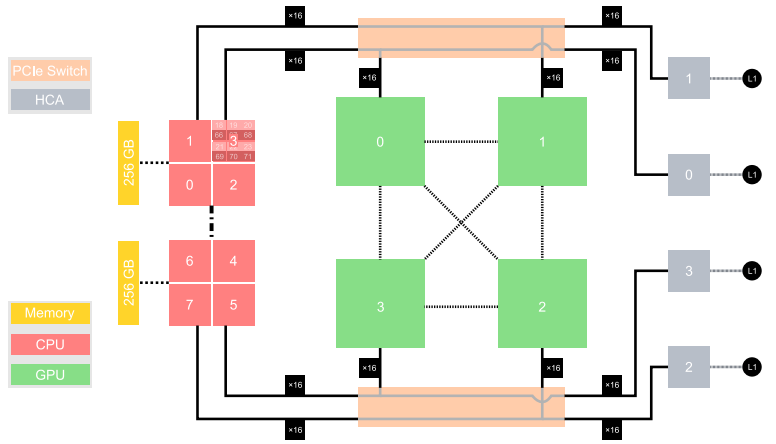

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Very valuable experience and an important part of working on research software targeting HPC systems.

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Long-term support with vexing JUWELS Booster node crashes

This situation and the way it was handled by the team at JSC convinced me to prepare this talk.

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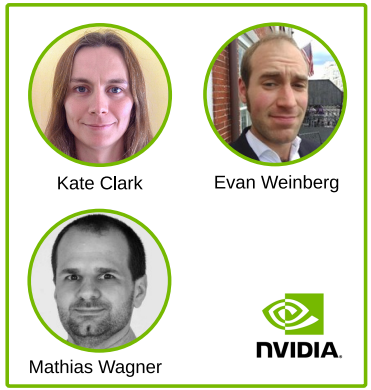
Didn't expect to find a CPU bug :)

Close interaction with support teams essential with these complicated HPC systems!

Thanks to everyone involved!



…and many others who have contributed explicitly or implictly!