RBC/UKQCD Computing overview

Towards CCP-TEPP

School of Physics and Astronomy
The University of Edinburgh

29/30 April 2025

THE UNIVERSITY *of* EDINBURGH

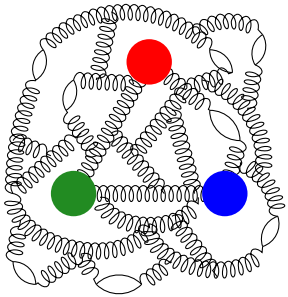
Supercomputing the strong nuclear force

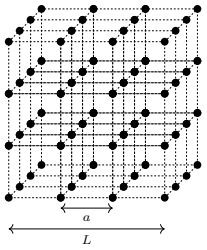
- Search for new physics to answer questions such as *What is dark matter?* or *What happened directly after the Big Bang?*
- strong nuclear force is one of the fundamental interactions in the Standard Model of Paricle Physics

  $\rightarrow$ at low energies quarks confined to hadrons

  $\rightarrow$ Monte Carlo Simulation

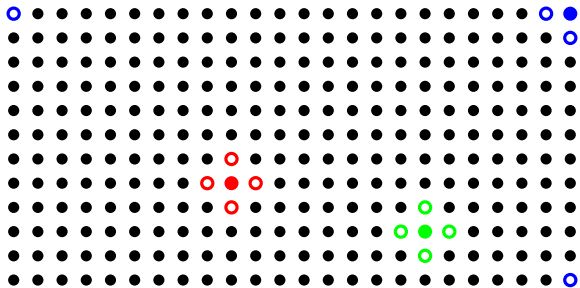
  $\rightarrow$ Lattice QCD
- aiming for unprecedented precision for, e.g., weak decays of hadrons, hadron spectroscopy & scattering, muon magnetic moment, ...





The Dirac operator on the lattice

- Solving the Dirac equation $\boldsymbol{D}\phi = \eta$
- (current) typical problem sizes: $\boldsymbol{D}$ is matrix of size $\sim \mathbf{10^9} \times \mathbf{10^9}$
  $\rightarrow$ solve numerically using Conjugate Gradient (CG)
- nearest neighbour interactions



$\rightarrow$ sparse matrix multiplication

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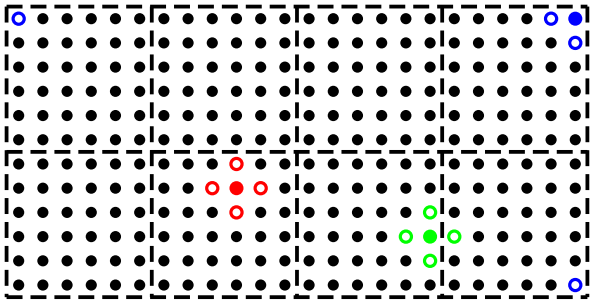
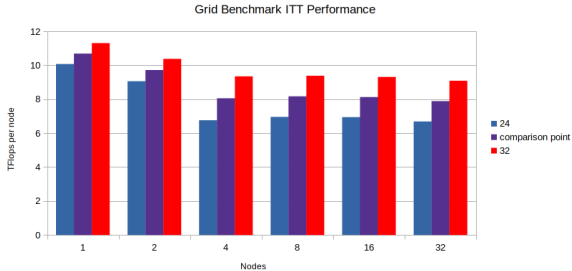


$\rightarrow$ sparse matrix multiplication
$\rightarrow$ halo exchange

Grid and Hadrons software packages

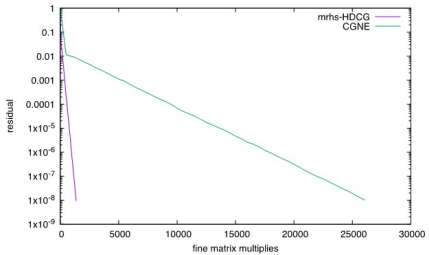
- software packages:
  - Grid
    `https://github.com/paboyle/Grid`
  - Hadrons `https://github.com/aportelli/Hadrons`



- perfect weak scaling from 4 to 32 nodes on DiRAC extreme scaling system Tursa
- high level data parallel approach: MPI, OpenMP and vector instructions
- high portability between many architectures, including GPU
- various different solvers and lattice actions

Algorithmic Developments

- Problem sizes enabled by Exascale require new algorithms
- **Recent**: solve multiple right-hand sides (mrhs) simultaneously and use GPU Tensor hardware
- physical quark masses, 18 nodes on Frontier (AMD MI250X):
  - Red-black preconditioned CG solves **single right-hand side in 770 s**
  - mrhs-HDCG solves **twelve right-hand sides in 1017 s**
  - total: **9.1× speed up**
  - 17× reduction in fine matrix multiplies



[Plot by P. Boyle]