

# Direct solves on a multigrid solver in lattice quantum chromodynamics (QCD)

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## Abstract

For our work we simulate spin- and color-charges in a 4-dimensional lattice using the Dirac-equation from quantum chromo dynamics (QCD). Here arises a large sparse linear system of equations which has to be solved. In order to solve this system as fast as possible we developed our own solver package based on several high performance algorithms over the years. Our solver uses an algebraic multigrid structure with domain-decomposition which allows us to shift the computational work from the original lattice to a much smaller one and simultaneously keeping the sparse structure intact. Since we perform a 4 dimensional simulation, this smaller lattice will consist of drastically less lattice points in comparison to the original one with an increased degree of freedom on each lattice point. But in the end, we greatly reduce the size of the sparse system of equations. This shift from one lattice to a much smaller, coarser one can be done several times, reducing the size of the linear system even further until we reach a final coarsest level, where we finally dare to perform a solve-step. At this point, MUMPS comes into play. On this coarsest level we use MUMPS to solve a system of about 250 000 equations directly. Our multigrid-method allows us to use very rough solutions on the coarsest level, which means we can use the block low rank feature of MUMPS for solve to reach a precision of up to  $10^{-1}$  or  $10^{-2}$ . Since the original fine lattice is very large our solver makes use of parallelism with MPI and openMP using a lot of processes. Restricting to the smaller coarser levels and therefore also smaller linear systems requires us to also reduce the number of active processes to keep a good balance of computation and communication for the entire solve. Using a smaller number of processes as the lattice and the linear system get restricted to smaller sizes is called "agglomeration" and therefore we use MUMPS still with MPI and openMP active but with a certainly smaller number of processes than the overall solve.