Simulation of full QCD using Overlap Fermions

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Most lattice Quantum Chromodynamics (QCD) formulations explicitly break chiral symmetry. This leads to unwanted mixing between operators of different chiral sectors, exceptional configurations when the simulated quark masses approach their physical values, and no clear definition of a topological index. The overlap Dirac operator solves these problems by satisfying a lattice variant of chiral symmetry, meaning that among the various lattice formulations used today, it is closest to the continuum Dirac operator. In particular, it has a well defined topological index which correctly accounts for the $U(1)$ anomaly. This makes overlap fermions the obvious choice when it comes to simulations focusing on topological properties of the vacuum of QCD, on observables sensitive to chiral symmetry breaking or phenomenology close to the physical quark masses.

However, using overlap fermions in practise is particularly challenging for two reasons: Firstly, they require a large amount of computer resources. The overlap Dirac operator contains the sign function of a large sparse matrix. As a consequence, inversions of the operator, required in any Hybrid Monte Carlo (HMC) algorithm or calculation of an observable, involve a two-level nested inversion. We have introduced new inversion algorithms accelerating this inversion by a factor of 10 \cite{Cundy2005}. Secondly, a HMC algorithm requires the differential of the sign function, leading to a delta function in the fermionic force. By treating small eigenvalues of the sparse matrix exactly and employing a reflection/transmission algorithm we have constructed a HMC algorithm which has high acceptance, good scaling with the lattice volume and quark mass, and conserves energy up to $O(\Delta t^2)$ \cite{Cundy2005}.

With these new algorithms and the Blue Gene/L supercomputer at NIC in Jülich - currently one of the most powerful systems worldwide - we can now generate full QCD vacuum configurations with overlap fermions. The Blue Gene/L has proven to be an architecture particularly well suited for QCD applications. It features a 3d torus network and a dual core node, matching the 4d torus topology of QCD. Additionally, the CPUs feature interconnected dual FPU, optimized for complex number calculations. The most time consuming parts of the code have been tuned using inline assembler or compiler intrinsic functions. Almost perfect scaling was achieved for fixed global problem size, while the scaling with fixed problem size per CPU is perfectly linear.

Several ensembles have been generated so far. These include configurations with lattice sizes of $32 \times 8^3$ and $16 \times 8^3$ and quark masses of 120, 160 and 200 MeV. These configurations are used to study the QCD vacuum and to investigate the nature of the topological objects in the gauge field which are believed to drive spontaneous chiral symmetry and (possibly) confinement \cite{Cundy2006}.

REFERENCES

2. N. Cundy et al., Numerical methods for the QCD overlap operator, hep-lat/0502007.

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