

FermiQCD: A tool kit for parallel lattice QCD applications

[<http://latticeqcd.fnal.gov/software/fermiqcd/>]

Massimo Di Piero^{a*}

^a Fermilab, Kirk and Pine St., Batavia, Illinois 60563, USA

We present here the most recent version of FermiQCD, a collection of C++ classes, functions and parallel algorithms for lattice QCD, based on Matrix Distributed Processing. FermiQCD allows fast development of parallel lattice applications and includes some SSE2 optimizations for clusters of Pentium 4 PCs.

1. Introduction

FermiQCD is a collection of classes, functions and parallel algorithms for lattice QCD [1], written in C++. It is based on Matrix Distributed Processing² (MDP) [2]. The latter is a library that includes C++ methods for matrix manipulation, advanced statistical analysis (such as Jackknife and Bootstrap) and optimized algorithms for interprocess communications of distributed lattices and fields. These communications are implemented using Message Passing Interface (MPI) but MPI calls are hidden to the high level algorithms that constitute FermiQCD.

FermiQCD works also on single processor computers and, in this case, MPI is not required.

2. FermiQCD overview

The basic fields defined in FermiQCD are:

class gauge_field:

List of implemented algorithms:

- heatbath algorithm
- anisotropic heatbath
- $O(a^2)$ heatbath

These algorithms work for arbitrary gauge groups $SU(N_c)$, for arbitrary lattice dimensions and topologies. FermiQCD also supports arbitrarily

twisted boundary conditions for large β computations and studies of topology.

class fermi_field:

List of implemented algorithms:

- multiplication by $Q = (\not{D} + m)$, for Wilson and Clover actions, for isotropic and anisotropic lattices
- minimal residue inversion for Q
- stabilized biconjugate gradient (BiCGStab) inversion for Q
- Wupperthal smearing for the field
- stochastic propagators

These algorithms work for arbitrary gauge groups $SU(N_c)$ and for arbitrary topologies in 4 dimensions. The multiplication by Q , clover (isotropic and anisotropic), for $SU(3)$, is optimized using Pentium 4 SSE2 instructions in assembler language. This implementation is based on the assembler macro functions written by Martin Lüscher [3]

class fermi_propagator:

This is an implementation of ordinary quark propagators. A `fermi_propagator` can be generated using any of the inversion algorithms of a `fermi_field`.

class staggered_field:

Kogut-Susskind (KS) fermion. List of implemented algorithms:

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²<http://www.phoenixcollective.org/mdp>

- multiplication by Q , for unimproved and $O(a^2)$ (Asqtad) improved actions [4]
- BiCGStab inversion for Q
- BiCGStab inversion for Q using the UML decomposition [5]
- function `make_meson`

These algorithms work for arbitrary gauge groups $SU(N_c)$ and for an arbitrary even number of dimensions (except `make_meson`). The multiplication by Q , both improved and unimproved, for $SU(3)$, is optimized using Pentium 4 SSE2 instructions in assembler language. In the unimproved case only half of the SSE2 registries are used and there is room for an extra factor two in speed. The function `make_meson` builds any meson propagator (made out of staggered quarks) for arbitrary $\text{Spin} \otimes \text{Flavour}$ structure. This algorithm is described in ref. [6]

class staggered_propagator:

This is an implementations of the staggered propagator consisting of 16 sources contained in a 2^4 hypercube at the origin of the lattice. A `staggered_propagator` can be used to propagate any hadron from the hypercube at the origin of the lattice to any other hypercube without extra inversions.

All fields in FermiQCD inherit the standard I/O methods of MDP (`save` and `load`) and the file format is independent on the lattice partitioning over the parallel processes. These I/O functions, as well as all the FermiQCD algorithms, are designed to optimize interprocess communications.

3. Example

We present here, as an example, a full program that generates 100 $SU(3)$ gauge configurations (U), starting from a hot one. On each configuration it computes a pion propagator (`pion`) made of $O(a^2)$ improved quark propagators and prints it out. These propagators are computed using the SSE2 optimized clover action and the BiCGStab inversion algorithm. The program works in parallel.

```

#define PARALLEL
#include "fermiqcd.h"

void main(int argc, char **argv) {
    mpi.open_wormholes(argc, argv);

    int t,a,b,conf;
    int nc=3, box[4]={16,8,8,8};
    generic_lattice L(4,box);
    gauge_field      U(L,nc);
    fermi_propagator S(L,nc);
    site             x(L);
    float            pion[16];
    U.param.beta=5.7;
    S.param.kappa=0.1345;
    S.param.cSW=1.5;

    default_fermi_action=
                                mul_Q_Luscher;
    default_inversion_method=
                                BiCGStab_inversion;

    set_hot(U);
    heatbath(U,100);
    for(conf=0; conf<100; conf++) {
        heatbath(U,30);
        compute_em_field(U);
        generate(S,U);
        for(t=0; t<16; t++) pion[t]=0;
        forallsites(x)
            for(a=0; a<4; a++)
                for(b=0; b<4; b++)
                    pion[x(TIME)]+=
                        real(trace(S(x,a,b)*
                                hermitian(S(x,b,a)))));
        mpi.add(pion, 16);
        if(ME==0) for(t=0; t<16; t++)
            printf("%i %f\n", t, pion[t]);
    }
    mpi.close_wormholes();
}

```

Comments:

- L is the user-defined name of the lattice (16×8^3)

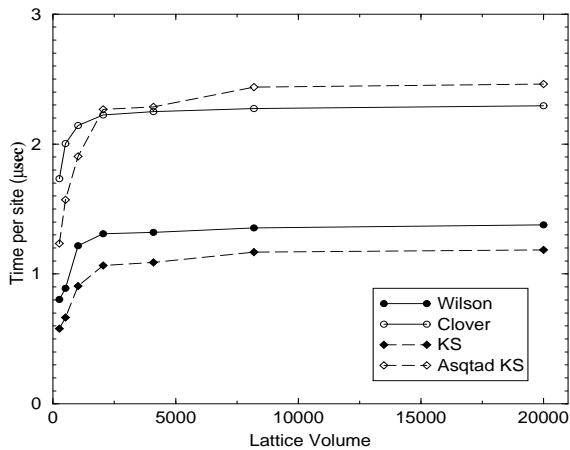


Figure 1. Time per site in μsec for `mul_Q_Luscher` (Wilson, clover, KS and Asqtad KS in single precision).

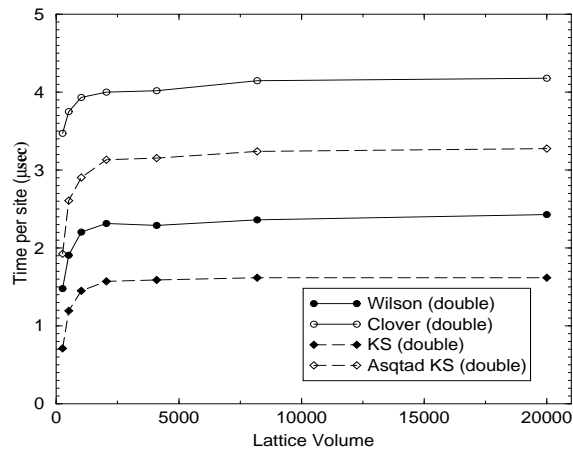


Figure 2. Time per site in μsec for `mul_Q_Luscher` (Wilson, clover, KS and Asqtad KS in single precision).

- `U`, `S` and `x` are the gauge field, the fermi propagator and an auxiliary `site` variable defined on the lattice `L`
- `default_fermi_action` is a pointer to the function that implements the action to be used. `mul_Q_Luscher` is one of the built-in clover actions, optimized for Pentium 4.
- `default_inversion_method` is a pointer to the function that implements the inversion algorithm (minimal residue or BiCGStab)
- `compute_em_field` computes the chromo-electro-magnetic field required by the action³.
- `generate` computes the quark propagator `S` on the given gauge configuration `U`.
- `forallsites(x)` is a parallel loop on `x`. Each processor loops on the local sites.
- `mpi.add(pion,16)` sums the vector `pion[16]` in parallel.

³The chromo-electro-magnetic field is a member variable of the gauge field. FermiQCD has almost no global variables except pointers to the functions that implement the algorithms.

- `if (ME==0)` guarantees that only one processor performs the output.

4. Benchmarks

In fig. 1 and fig. 2 we report some benchmarks for the multiplication by Q of a fermionic field, for the different actions (using a single CPU Pentium 4 PC running at 1.4 GHz, Linux 2.4 and gcc 2.95.3).

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REFERENCES

1. M. Di Pierro, hep-lat/0009001. (Lattice QCD tutorial with examples in FermiQCD)
2. M. Di Pierro, hep-lat/0004007. (Updated tutorial on MDP) To be published on CPC.
3. M. Lüscher, *these proceedings*
4. G. P. Lepage, Phys.Rev. D59 (1999) 074502
5. K. Orginos *et al.* (MILC), Phys.Rev. D59 (1999) 014501
6. M. Di Pierro, *in preparation*