

[www.fermiqcd.net](http://www.fermiqcd.net)

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## 1. INTRODUCTION

FermiQCD[1][2] is a C++ library for fast development of parallel lattice QCD applications. The expression FermiQCD Collaboration is used as a collective name to indicate both the users of the software and its contributors.

One of the main differences between FermiQCD and libraries developed by other collaborations is that it follows an object oriented design as opposed to a procedural design. FermiQCD should not be identified exclusively with the implementation of the algorithms but, rather, with the strict specifications that define its Application Program Interface. One should think of FermiQCD as a language on its own (a superset of the C++ language), designed to describe Lattice QCD algorithms. The objects of the language include complex numbers (`mdp_complex`), matrices (`mdp_matrix`), lattices (`mdp_lattice`), fields (`gauge_field`, `fermi_field`, `staggered_field`), propagators (`fermi_propagator`) and actions. Algorithms written in terms of these objects are automatically parallel.

Some of the advantages of our design approach are the following:

- Programs written in FermiQCD are easy to write, read and modify since the FermiQCD syntax resembles the mathematical syntax used in Quantum Field Theory articles and

books.

- Programs are portable in the sense that they can, in principle, be compiled with any ANSI C++ compiler. Hardware specific optimizations are coded in the library and hidden from the high level programmer.
- The high level programmer does not have to deal with parallelization issues since the underlying objects deal with it. FermiQCD communications are based on MPI.
- Programs are easier to debug because the usage of FermiQCD objects and algorithms does not require explicit use of pointers. All memory management is done by the objects themselves.

FermiQCD was originally designed with one main goal in mind: easy of use. It is true that in many cases this requires a compromise with speed. For example, FermiQCD actions and fields support arbitrary  $SU(n_c)$  gauge group and it is not practical to optimize the linear algebra for any  $n_c$ . However it is convenient to optimize some of the specific cases of interest (such as  $n_c = 3$ ) while maintaining compatibility with the FermiQCD syntax. At present the FermiQCD library includes multiple implementations of each action (Wilson, Clover, Kogut-Susskind, Asqtad[3], Domain Wall, Fermilab[4])

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and, for each action, at least one implementation is optimized for  $SU(3)$ . In particular, we provide a FermiQCD port of the Clover  $SU(3)$  action coded by M. Lüscher using SSE assembly instructions for Pentium 4[5].

The following code declares two fermionic fields (`phi` and `psi`) and one  $SU(nc)$  gauge field (`U`) on a given lattice (`lattice`), reads `psi` and `U` from disk and computes

$$\varphi = Q[U, \kappa]^{-1} \psi$$

where  $Q[U, \kappa] = D[U] + m[\kappa]$  is the Dirac matrix and  $\kappa$  is the typical lattice parameter that sets the mass scale:

```
fermi_field phi(lattice, nc);
fermi_field psi(lattice, nc);
gauge_field U(lattice, nc);
coefficients light_quark;
psi.load("fermi_field.mdp");
U.load("gauge_field.mdp");
light_quark["kappa"]=0.123;
if(nc==3) default_fermi_action=
    FermiCloverActionSSE2::mul_Q;
mul_invQ(phi, psi, U, light_quark);
```

Note that when  $nc = 3$  the above program uses the SSE optimized Wilson action. If  $nc \neq 3$  a different implementation of the Wilson action is used. FermiQCD programs are transparent to the choice of the action.

On a cluster of 2GHz Pentium 4 PCs connected by Myrinet, one double precision  $SU(3)$  minimum residue step with Clover action takes 4.8 micro seconds per lattice site. The efficiency drops to 75 – 80% on 8 processors. For more benchmarks we refer to the [www.fermiqcd.net](http://www.fermiqcd.net) web page.

FermiQCD programs are implicitly parallel. Each lattice object determines an optimal communication pattern for its sites assuming a next-neighbor, a next-next-neighbor or a next<sup>3</sup>-neighbor interaction in the action. The optimal patterns are determined according to empirical rules that minimize dependence on the network latency and minimize communication load.

## 2. EXAMPLES

### 2.1. Computing the average plaquette

Given a  $\mu\nu$ -plane, the average plaquette, for each gauge configuration, is defined as

$$\langle P_{\mu\nu} \rangle = \frac{1}{V} \text{ReTr} \sum_x U_\mu(x) U_\nu(x + \hat{\mu}) \quad (1)$$

$$[U_\nu(x) U_\mu(x + \hat{\nu})]^H \quad (2)$$

here is the corresponding FermiQCD syntax:

```
forallsites(x)
    p=p+real(trace(U(x,mu)*U(x+mu,nu)*
        hermitian(U(x,nu)*U(x+nu,mu)))));
p=p/lattice.size();
```

In the above code `forallsites` is a parallel loop,  $U(x, \mu)$  is  $n_c \times n_c$  color matrix.

### 2.2. Implementing the Dirac-Wilson action

As another example, we consider here the following Wilson discretization of the Dirac action:

$$\varphi_\alpha = \psi_\alpha - \kappa \sum_\mu (1 + \gamma_\mu)_{\alpha\beta} U_\mu(x) \psi_\beta(x + \hat{\mu}) + \quad (3)$$

$$(1 - \gamma_\mu)_{\alpha\beta} U_\mu^H(x - \hat{\mu}) \psi_\beta(x - \hat{\mu}) \quad (4)$$

which can be translated into the following FermiQCD code:

```
phi=psi;
forallsites(x)
    for(int mu=0; mu<4; mu++) {
        for(int b=0; b<4; b++) {
            psi_up(b)=U(x,mu)*psi(x+mu,b);
            psi_dw(b)=hermitian(U(x-mu,mu))*
                psi(x-mu,b);
        }
        phi=phi-kappa*((1+Gamma[mu])*psi_up+
            (1-Gamma[mu])*psi_dw);
    }
```

Note how “1” in this context is interpreted as a diagonal unitary matrix. The sum on  $\alpha$  is implicit since `psi_up` and `psi_dw` are spin $\times$ color matrices.

### 2.3. Computing the pion propagator

The pion propagator is defined as

$$C_2(x_0) = \sum_{x_1, x_2, x_3} \langle \pi(x) \pi(0) \rangle \quad (5)$$

$$= \text{ReTr} \sum_{x_1, x_2, x_3} \sum_{\alpha, \beta} S_{\alpha\beta}(x) S_{\beta\alpha}^H(x) \quad (6)$$

where  $S$  is a light quark propagator in the background gauge field  $U$ :

$$S_{\alpha\beta}^{ij}(x) = \int [dq d\bar{q}] q(x) \bar{q}(0) e^{Action[q,U]} \quad (7)$$

Here is the FermiQCD syntax for Eq. (6):

```
generate(S,U,light_quark);
forallsites(x)
  for(int a=0; a<4; a++)
    for(int b=0; b<4; b++)
      C2(x(0))+=real(trace(S(x,a,b)*
        hermitian(S(x,b,a))));
```

where  $S(x,a,b)$  is a color $\times$ color matrix. The function `generate` creates the propagator  $S$  by calling the inverter (for example the minimum residue or the stabilized bi-conjugate gradient). Each of the inverters works on any of the provided actions and also on user defined actions.

### 3. CONCLUSIONS

In our experience the cost of developing and debugging software is one of the major costs of Lattice QCD computations. FermiQCD was designed to standardize this software development process and, therefore, reduce the cost for the community.

FermiQCD comes in the form of a library (with examples), rather than a collection of ready made programs, since we understand that different research groups have different requirements. Some ready made programs for specific computations (such as generating gauge configurations, computing meson propagators, etc.) are available as examples, while others are available upon request to the authors. We provide converters for the most common data formats including UKQCD, MILC, CANOPY and various binary formats.

The FermiQCD libraries can be used freely for research purposes and we do not require that users share their programs unless they wish to do so (although we feel that this practice should be encouraged).

On one hand, FermiQCD is a mature project. The present implementation has been tested independently by different groups and it has been

used to develop large scale lattice QCD computations. On the other hand, there is a lot of work that needs to be done, including:

- implementing dynamical fermions
- developing a graphical interface
- optimizing the gauge actions
- porting the low level communications libraries (currently based on MPI) to other protocols such as TCP/IP for Gigabit ethernet and SciDAC API for the QCDOC.
- incorporating grid-like features, including the ability to read and write data in the new international data grid standard for gauge configurations.
- implementing new actions such as the Iwasaki gauge action and Overlap fermions.
- building a collection of ready-to-use programs and related documentation.

The development of FermiQCD has greatly benefited from access to other codes such as UKQCD (from which we borrowed the local random number generator), MILC (for the staggered fermion algorithms), CANOPY (for many design features), M. Lüscher's (for the assembly macros) and C. Michael's (for all-to-all propagators); we thank their authors for making them available to us. We also wish to thank J. Flynn, A. Shams, F. Mescia, L. Del Debbio and T. Rador for their through tests of the inverters and the Clover action.

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