A Linux PC cluster for lattice QCD with exact chiral symmetry

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Abstract

A computational system for lattice QCD with overlap Dirac quarks is described. The platform is a home-made Linux PC cluster, built with off-the-shelf components. In the initial phase, this system constitutes of 30 nodes, with each node consisting of one Pentium 4 processor (1.6/2.0 GHz), one Gbyte of PC800 RDRAM, one 40/80 Gbyte hard disk, and a network card. The computationally intensive parts of our program are written in SSE2 codes. The speed of this system is estimated to be 30 Gflops, and its price/performance is better than $1.0/Mflops for 64-bit (double precision) computations in quenched QCD. We discuss how to optimize its hardware and software for computing propagators of overlap Dirac quarks.

PACS numbers: 11.15.Ha, 11.30.Rd, 12.38.Gc
Keywords: Lattice QCD, Overlap Dirac quarks, Linux PC cluster
1 Introduction

Our objective is to extract physics from lattice QCD with possibly minimal amount of computations. Obviously, the required computing power exceeds that of any desktop personal computer currently available in the market. Thus, for one without supercomputer resources, building a computational system [1] seems to be inevitable if one really wishes to pursue a meaningful number of any physical quantity from lattice QCD. However, the feasibility of such a project depends not only on the funding, but also on the theoretical advancement of the subject, namely, the realization of exact chirally symmetry on the lattice [2, 3]. Now, if we also take into account of the current price/performance of PC hardware components (CPU + RAM + hard disk\(^1\)), it seems to be the right timing to rejuvenate the project [1] with a new goal - to build a computational system for lattice QCD with exact chiral symmetry. In this paper, we outline the essential features of a Linux PC cluster which is now being developed at National Taiwan University. In particular, we discuss how to optimize its hardware and software for lattice QCD with overlap Dirac quarks.

First, we start from quenched QCD calculations (i.e., ignoring any internal quark loops by setting \(\text{det} D = 1\)). Thus, our first task is to compute quark propagators in the gluon field background, for a sequence of configurations generated stochastically with weight \(\exp(-A_g)\) (\(A_g\) : pure gluon action). Then the hardronic observables such as meson and baryon correlation functions can be constructed, and from which the hadron masses and decay constants can be extracted. We use the Creutz-Cabbibo-Marinari heat bath algorithm [4, 5] to generate ensembles of \(SU(3)\) gauge configurations.

The computation of quark propagators depends on the scheme of lattice fermions, the hard core of lattice QCD. In general, one requires that any quark propagator coupling to physical hadrons must be of the form [6]

\[
(D_c + m_q)^{-1},
\]

(1)

where \(m_q\) is the bare quark mass, and \(D_c\) is a chirally symmetric and anti-hermitian Dirac operator \([D_c\gamma_5 + \gamma_5 D_c = 0 \text{ and } (iD_c)^\dagger = iD_c]\). Here we assume that \(D_c\) is doubler-free, has correct continuum behavior, and \(D = D_c(1 + r a D_c)^{-1}\) is exponentially local for a range of \(r > 0\). Note that the way \(m_q\) coupling to \(D_c\) is the same as that in the continuum. The chiral symmetry of \(D_c\) (even at finite lattice spacing) is the crucial feature of any quark coupling to physical hadrons. Otherwise, one could hardly reproduce the low energy strong interaction phenomenology from lattice QCD.

For any massless lattice Dirac operator \(D\) satisfying the Ginsparg-Wilson relation [7]

\[
D\gamma_5 + \gamma_5 D = 2raD\gamma_5 D,
\]

(2)

it can be written as [8]

\[
D = D_c(1 + r a D_c)^{-1},
\]

and the bare quark mass is naturally added to the \(D_c\) in the numerator [6],

\[
D(m_q) = (D_c + m_q)(1 + r a D_c)^{-1}.
\]

\(^1\)The emergence of low-price and high-capacity ( > 40 Gbyte ) IDE hard disk turns out to be also rather crucial for this project, since the data storage is enormous.
Then the quenched quark propagator becomes

\[(D_c + m_q)^{-1} = (1 - rm_qa)^{-1}[D(m_q)^{-1} - ra] \tag{3}\]

If we fix one of the end points at \((\vec{0}, 0)\) and use the Hermiticity \(D^\dagger = \gamma_5D\gamma_5\), then only 12 (3 colors times 4 Dirac indices) columns of

\[D(m_q)^{-1} = D^\dagger(m_q)\{D(m_q)D^\dagger(m_q)\}^{-1} \tag{4}\]

are needed for computing the time correlation functions of hadrons. Now our problem is how to optimize a PC cluster to compute \(D(m_q)^{-1}\) for a set of bare quark masses.

The outline of this paper is as follows. In Section 2, we briefly review our scheme of computing propagators of overlap Dirac quark. The details have been given in Ref. [9]. In Section 3, we discuss a simple scheme of memory management for the nested conjugate gradient loops. In Section 4, we discuss how to implement the SSE2 codes for the computationally intense parts of our program. In Section 5, the performance of our system is measured in terms of a number of tests pertaining to the computation of overlap Dirac quark propagators. In Section 6, we conclude with some remarks and outlooks.

## 2 Computational Scheme for overlap Dirac quarks

The massless overlap Dirac operator [2] reads as

\[D = m_0a^{-1}\left(1 + \gamma_5\frac{H_w}{\sqrt{H_w^2}}\right) \tag{5}\]

where \(H_w\) denotes the Hermitian Wilson-Dirac operator with a negative parameter \(-m_0\),

\[H_w = \gamma_5D_w = \gamma_5(-m_0 + \gamma_\mu t_\mu + W),\]

\(\gamma_\mu t_\mu\) the naive fermion operator, and \(W\) the Wilson term. Then \(D\) (5) satisfies the Ginsparg-Wilson relation (2) with \(r = 1/(2m_0)\). In this paper, we always fix \(m_0 = 1.3\) for our computations. Details of our implementation for computing overlap Dirac quark propagators have been given in Ref. [9].

Basically, we need to solve the following linear system

\[D(m_q)D^\dagger(m_q)Y = \begin{cases} m_q^2 + \left(2m_0^2 - \frac{m_q^2}{2}\right) \left[1 + \frac{(\gamma_5 \pm 1)}{2}H_w\frac{1}{\sqrt{H_w^2}}\right] \end{cases} Y = I \tag{7}\]

by conjugate gradient (CG). Then the quark propagators can be obtained through (4). With Zolotarev optimal rational approximation [10, 11, 12, 13] to \((H_w^2)^{-1/2}\), the multiplication\(^2\)

\[H_w\left(\frac{1}{\sqrt{H_w^2}}\right)Y, \quad h_w \equiv \frac{H_w}{\lambda_{\text{min}}} \]

\[\simeq h_w(h_w^2 + c_{2n})\sum_{l=1}^{n} \frac{b_l}{h_w^2 + c_{2l-1}}Y = h_w(h_w^2 + c_{2n})\sum_{l=1}^{n} b_lZ_l \tag{8}\]

\(^2\)Note that the Zolotarev optimal rational polynomial in Eq. (8) is in the form \(r^{(n,n)}\) which is different from \(r^{(n-1,n)}\) used in Ref. [9]. We refer to Ref. [13] for further discussions.
can be evaluated by invoking another conjugate gradient process to the linear systems

\[ (h_w^2 + c_{2l-1})Z_l = Y, \quad l = 1, \ldots, n. \]  

(9)

where

\[
\begin{align*}
  c_l &= \frac{\text{sn}^2\left(\frac{lK'}{2n+1}; \kappa'\right)}{1 - \text{sn}^2\left(\frac{lK'}{2n+1}; \kappa'\right)} \\
  b_l &= d_0 \frac{\prod_{i=1}^{n-1} (c_{2i} - c_{2l-1})}{\prod_{i=1, i \neq l}^{n} (c_{2i-1} - c_{2l-1})} \\
  d_0 &= \frac{2\lambda}{1 + \lambda} \prod_{l=1}^{n} (1 + c_{2l-1}) \prod_{l=1}^{2n+1} \Theta\left(\frac{2K'}{2n+1}; \kappa'\right) \\
  \lambda &= \frac{2n+1}{\prod_{l=1}^{\Theta\left((2l-1)K'; \kappa'\right)}}.
\end{align*}
\]

Here \( \Theta \) denotes the elliptic theta function, and the Jacobian elliptic function \( \text{sn}(u; \kappa') \) is defined by the elliptic integral

\[ u = \int_0^{\text{sn}} \frac{dt}{\sqrt{(1 - t^2)(1 - \kappa'^2t^2)}}, \]

and \( K' \) is the complete elliptic integral of the first kind with modulus \( \kappa' \),

\[ K' = \int_0^1 \frac{dt}{\sqrt{(1 - t^2)(1 - \kappa'^2t^2)}}, \]

where \( \kappa' = \sqrt{1 - 1/b} \), \( b = \lambda_{\text{max}}^2/\lambda_{\text{min}}^2 \), and \( \lambda_{\text{max}}^2 \) and \( \lambda_{\text{min}}^2 \) are the maximum and the minimum of the eigenvalues of \( H_w^2 \).

Instead of solving each \( Z_l \) individually, one can use multi-shift CG algorithm [14, 15], and obtain all \( Z_l \) altogether, with only a small fraction of the total time what one had computed each \( Z_l \) separately. Evidently, one can also apply multi-shift CG algorithm to (7) to obtain several quark propagators with different bare quark masses.

In order to improve the accuracy of the rational approximation as well as to reduce the number of iterations in the inner CG loop, it is crucial to narrow the interval \([1, b]\) by projecting out the largest and some low-lying eigenmodes of \( H_w^2 \). We use Arnoldi algorithm [16] to project these eigenmodes. Denoting these eigenmodes by

\[ H_wu_j = \lambda_j u_j, \quad j = 1, \ldots, k, \]  

(10)

then we project the linear systems (9) to the complement of the vector space spanned by these eigenmodes

\[ (h_w^2 + c_{2l-1})\tilde{Z}_l = \tilde{Y} \equiv (1 - \sum_{j=1}^{k} u_j u_j^\dagger)Y, \quad l = 1, \ldots, n. \]  

(11)
In the set of projected eigenvalues of $H^2_w$, \{\lambda^2_j, j = 1, \ldots, k\}, we use $\lambda^2_{\text{max}}$ and $\lambda^2_{\text{min}}$ to denote the least upper bound and the greatest lower bound of the eigenvalues of $\bar{H}^2_w$, where

$$\bar{H}_w = H_w - \sum_{j=1}^{k} \lambda_j u_j u_j^\dagger.$$  

Then the eigenvalues of

$$h^2_w = \bar{H}^2_w / \lambda^2_{\text{min}}$$

fall into the interval $(1, b)$, $b = \lambda^2_{\text{max}} / \lambda^2_{\text{min}}$.

Now the matrix-vector multiplication (8) can be expressed in terms of the projected eigenmodes (10) plus the solution obtained from the conjugate gradient loop (11) in the complementary vector space, i.e.,

$$H_w \frac{1}{\sqrt{H^2_w}} Y \simeq \frac{1}{\lambda_{\text{min}}} H_w (h^2_w + c_{2n}) \sum_{l=1}^{n} b_l \bar{Z}_l + \sum_{j=1}^{k} \lambda_j \sqrt{\lambda^2_j} u_j u_j^\dagger Y \equiv S$$

Then the breaking of exact chiral symmetry (2) can be measured in terms of

$$\sigma = \frac{|S^\dagger S - Y^\dagger Y|}{Y^\dagger Y}.$$  

In practice, one has no difficulties to attain $\sigma < 10^{-12}$ for most gauge configurations on a finite lattice [13].

Now the computation of overlap Dirac quark propagators involves two nested conjugate gradient loops: the so-called inner CG loop (11), and the outer CG loop (7). The inner CG loop is the price what one pays for preserving the exact chiral symmetry at finite lattice spacing.

### 3 Memory management

In this section we discuss how to configure the hardware and software of a PC cluster such that it can attain the optimal price/performance for the execution of the nested CG loops, (7) and (11).

First, we examine how much memory is required for computing one of the 12 columns of the quark propagators for a set of bare quark masses, since each column can be computed independently. If the required memory can be allocated in a single node, then each node can be assigned to work on one of the 12 columns of the quark propagators. Then the maximum speed of a PC cluster is attained since there is no communication overheads. Nevertheless, the memory (RDRAM) is the most expensive component, thus its amount should be minimized even though the maximum memory at each node can be up to 4 Gbyte. On the other hand, if one distributes the components of the nested CG loops across the nodes and performs parallel computations (with MPI) through a fast network switch, then the memory at each node can be minimal. However, the cost of a fast network switch and its accessories is rather expensive, and also the efficiency of the entire system will be greatly reduced due to the communication overheads.
overheads. Therefore, to optimize the price/performance of the PC cluster relies on what is the minimal memory required for computing one of the 12 columns of the quark propagators.

Let \( N_s = L^3 \times T \) denote the total number of lattice sites, then each column of \( D^{-1} \) with double complex (16 bytes) entries takes

\[
N_v = N_s \times 12 \times 16 \text{ bytes.} \tag{14}
\]

Using \( N_v \) or one column as the unit, we list the memory space of all components during the execution of the nested CG loops:

- Gauge links: 3.
- Number of projected low-lying eigenmodes: \( k \)
- Quark propagators \([\text{i.e., } Y \text{ in (7)}]\) of \( N_m \) masses: \( N_m/2 \).
  (Note that each \( Y \) only takes 1/2 column since it is chiral.)
- Conjugate gradient vectors in the CG algorithm: \( N_m/2 \).
- Residual vector for the outer CG loop: 1/2.
- The vector \( \bar{Y}_1 \) (of the smallest bare quark mass) at the interface between the inner and the outer CG loops: 1.
- The inner CG loop: \( 2n + 3 \) (where \( n \) is the degree of Zolotarev rational polynomial), which consists of
  (i) \( \{Z_i\} \) vectors: \( n \);
  (ii) Conjugate gradient vectors \( \{w_l\} \): \( n \);
  (iii) Residual vector (\( r \)): 1;
  (iv) \( H_w |w_1\rangle : 1 \);
  (v) \( H_2^w |w_1\rangle : 1 \).

Therefore, the memory space for all components of the nested CG loops is

\[
N_{cg} = (N_m + 1/2) + (2n + 3) + k + 3 = N_m + 2n + k + 6.5 \text{ (columns)} \tag{15}
\]

A schematic diagram of all components of the nested CG loops is sketched in Fig. 1.

Suppose we wish to compute overlap Dirac quark propagators on the \( 16^3 \times 32 \) lattice (at \( \beta = 6.0 \)), with parameters \( k = 16 \), \( n = 16 \), and \( N_m = 16 \). Then, according to (14) and (15),

\[
N_v \simeq 0.024 \text{ Gbyte,} \quad N_{cg} = 70.5 \text{ columns,}
\]

the required memory for all components of the nested CG loops is

\[ N_{cg} \times N_v \simeq 70.5 \times 0.024 = 1.7 \text{ Gbyte} \]

This seems to imply that one should install\(^3\) four stripes of 512 Mbyte modules (i.e. total 2 Gbyte) at each node, if one wishes to let each node compute independently, and to attain

\(^3\)At present, most Pentium 4 motherboards designed for housing PC800 RDRAM have 4 memory slots.
the maximum speed of the PC cluster. However, this is a rather expensive solution at this moment, in view of the current price of 512 Mbyte modules. On the other hand, if one distributes the components of the nested CG loops across the nodes and performs parallel computations (with MPI) through a fast network switch, then the price/performance seems to be even worse than the former solution.

Fortunately, we observe that not all column vectors are used simultaneously at any step of the nested CG loops, and also the computationally intense part is at the inner CG loop. Thus we can use the hard disk as the virtual memory for the storage of the intermediate solution vectors and their conjugate gradient vectors \( Y_\sigma, P_\sigma, \sigma = 1, \ldots, N_m \) at each iteration of the outer CG loop, while the CPU is working on the inner CG loop. Then the minimal physical memory required at each node can be greatly reduced. Also, the projected eigenmodes are not required to be kept inside the memory, since they are only needed at the start of the inner CG loop to compute \( \bar{Y}_1 \) (for the smallest bare quark mass),

\[
\bar{Y}_1 \equiv (1 - \sum_{j=1}^{k} u_j u_j^\dagger) Y_1 ,
\]

and

\[
\sum_{j=1}^{k} \frac{\lambda_j}{\sqrt{\lambda_j}} u_j u_j^\dagger Y_1 \equiv \varepsilon_p Y_1
\]

where \( \varepsilon_p Y_1 \) is only needed for computing \( S(12) \) at the completion of the inner CG loop. Thus one has the options to keep the vector \( \varepsilon_p Y_1 \) inside the memory during the entire inner CG loop or save it to the hard disk and then retrieve it at the completion of the inner CG loop. Further, since \( \bar{Y}_1 \) is only needed at the start of the inner CG loop, so it can share the same memory location with the residual vector \( r \).

Now it is clear that the minimum memory at each node (without suffering a substantial loss in the performance) is

\[
N_{\text{cg}}^{\text{min}} = (2n + 3) + 3 = 2n + 6 \text{ (columns)} ,
\]

which suffices to accommodate the link variables and all relevant vectors for the inner CG loop. After the completion of the inner CG loop and the vector \( S(12) \) is computed, the
memory space of $2n + 3$ column vectors is released, and the vectors $\{Y_\sigma\}$ and $\{P_\sigma\}$ of the outer CG loop can be read from the hard disk, which are then updated to new values according to the CG algorithm.

With this simple scheme of memory management, the minimal memory for computing one of the 12 columns of the quark propagators (for a set of bare quark masses) on the $16^3 \times 32$ lattice with $n = 16$ (degree of Zolotarev rational polynomial) becomes

$$N_{eg}^{min} \times N_v = 38 \times 0.024 = 0.912 \text{ Gbyte.}$$

Thus the computation can be performed at a single node with one Gbyte of memory, which can be implemented by installing four stripes of 256 Mbyte memory modules, a much more economic solution than using $4 \times 512$ Mbyte modules. Moreover, the time for disk I/O (at the interface of inner and outer CG loops) only constitutes a few percent of the total time for the execution of the entire nested CG loops (Table 3). This is the optimal memory configuration for a PC cluster to compute overlap Dirac quark propagators on the $16^3 \times 32$ lattice, which of course is not necessarily the optimal one for other lattice sizes. However, our simple scheme of memory management for the nested CG loops should be applicable to any lattice sizes, as well as to other systems.

In passing, we emphasize that the Zolotarev optimal rational approximation to $(H^2_w)^{-1/2}$ plays a crucial role to minimize the number of vectors required for the inner CG loop. If one had used other rational approximations, then it would require a very large $n$ to preserve exact chiral symmetry to a high precision (e.g., $\sigma < 10^{-11}$). In that case, it would be impossible to attain the optimal price/performance as what has been outlined above.

4 The SSE2 acceleration

With the optimal memory allocation for each node, we further enhance the performance of our lattice QCD codes (in Fortran) by rewriting its computationally intense parts in the SSE2 assembly codes of Pentium 4. In this section, we briefly review the basic features of the vector unit (SSE2) of Pentium 4, and then describe how to implement SSE2 codes in our lattice QCD program.

4.1 The basic features of SSE2

The simplest and the most efficient scheme of parallel computation is Single Instruction Multiple Data (SIMD). It can be implemented inside CPU through a set of long registers. If each register can accommodate several (say, $s$) data entries, then any operation (addition, subtraction, multiplication and division) on these registers will act on all data entries in parallel, thus yields the speed-up by a factor of $s$ comparing with normal registers. A schematic diagram is shown in Fig. 2.

Even though Intel had implemented the vector unit in their CPUs since Pentium-MMX series, only in the most recent IA-32 Pentium 4 and the advanced IA-64 Itanium, the architecture has been extended to SSE2 (Streamed SIMD Extension 2) to incorporate double precision data entries.
The Pentium 4 processor has eight registers (%xmm0, %xmm1, ..., %xmm7) for SIMD operations [18]. Each register is 128 bits wide and can accomodate 4 integers, or 4 single-precision or 2 double-precision floating point numbers. Since we always use double precision floating point numbers in our program, the execution speed of our program can be almost doubled if SSE2 is turned on judiciously in the computationally intensive parts. Note that SSE2 complies with the IEEE 32-bit and 64-bit arithmetic, thus the precision is lower than the extended 80-bit precision of the normal registers in Pentium 4. However, the difference is less than one part in $10^{15}$ (double precision), thus is negligible in our computations.

### 4.2 How to implement SSE2 codes in Fortran programs

Since our lattice QCD codes were originally written in Fortran 77, it would be natural if SSE2 codes can be directly embedded in our Fortran program. However, to our knowledge, the Fortran compilers currently available in the market do not support the option of inlining SSE2 codes. Moreover, for optimal performance of SSE2, the data should be aligned to 16-byte memory boundary. This can be easily carried out in C. Therefore our strategy to implement SSE2 codes is rewrite the main program unit in C such that the data arrays are allocated and aligned to 16 bytes memory boundary, then the SSE2 codes are embedded in C subroutines which are then called by original routines in Fortran.

Of course, if one has written lattice QCD codes in C, then the SSE2 codes can be embedded in C routines directly, without dealing with the interface of C and Fortran.

In the following, we illustrate our scheme of implementing SSE2 codes with an example program. The default compilers are gcc and g77 in Linux.

```
program main
implicit none
integer n
parameter (n=100)
double precision r(n), v(n)
call vxzero(n, r, v)
end

subroutine vxzero(n, r, v)
implicit none
```

![Figure 2: Double precision multiplication performed by the SSE2 instruction in the SIMD registers.](image)

![Table: SSE2 registers](table)
Here the Fortran main program calls the subroutine vxzero which in turn calls a computationally intensive routine vadd.

First, we rewrite the main program in C, with the data arrays allocated and properly aligned.

```c
#include <malloc.h>
int main(int argc, char **argv)
{
    int n=100;
    double *r, *v;
    /* setup the environment for Fortran */
    f_setarg(argc, argv);
    f_setsig();
    f_init();
    /* allocate r & v, and align them to 16-byte boundary */
    r = memalign(16, n*sizeof(double));
    v = memalign(16, n*sizeof(double));
    /* call the Fortran subroutine */
    vxzero_(&n, r, v);
    /* shutdown the I/O channels of Fortran */
    f_exit();
    exit(0);
    return 0;
}
```

The function call `memalign()` dynamically allocates 16 bytes aligned pointers r and v. Then the aligned arrays v[] and r[] can be passed to C subroutines for SSE2 operations.

Next we rewrite the computationally intensive routine vadd in C with embedded SSE2 codes.

```c
/* load variable a into %%xmm0 */
#define sse_load(a)  
    __asm__ __volatile__ ( "movapd %0, %%xmm0" :: "m" (a))

/* r = r + %%xmm0 x v */
#define sse_add(r, v)  
    __asm__ __volatile__ ( 
        "movapd %1, %%xmm1 \n\t"
        "movapd %0, %%xmm0" :: 
        "m" (a), 
        "m" (v))
```
"movapd %2, %xmm2 \n\t" \n"mulpd %xmm0, %xmm2 \n\t" \n"addpd %xmm1, %xmm2 \n\t" \n"movapd %xmm2, %0" \n:

/* store to address \(r\), which is indexed as \%0 */ \n"=m" (r) \n:

/* load from address \(r\) and \(v\), which are \nindexed as \%1 and \%2, respectively */ \n"m" (r), "m" (v))

#define ALIGN16 __attribute__ ((aligned (16)))

void vadd_(int *n, double *coeff, double *r, double *v)
{
    int i, len;
    static double cc[2] ALIGN16;

    /* the array \(cc\) is aligned to 16-byte boundary */

    cc[0] = cc[1] = *coeff;
    sse_load(cc[0]);
    len = (*n)/2;
    for (i=0; i<len*2; i+=2) {
        sse_add(r[i], v[i]);
    }
    if (*n % 2 != 0)
        r[len*2] = r[len*2] + cc[0] * v[len*2];
}

Note that we have added the keyword "volatile" (an GNU extension) in the macro "asm". Its purpose is to ensure that the compiler does not rearrange the order of execution of the codes during compilation. Finally, all object modules are linked by gcc with the option "-lsg2c".

4.3 The implementation of \(H_w \times |v\rangle\)

In our lattice QCD program, most of the execution time is spent in solving quark propagators via the nested CG loops. Thus the execution time is dominated by the operation \(H_w \times |v\rangle\), which is performed many times (\(> 10^5\) in most cases) before the final results of quark propagators can be obtained. Thus it is crucial to optimize this operation with SSE2 codes.

First, we have to set up the correspondence between the data structures used by C and Fortran routines in our program, in particular, for the link variables and the relevant vectors in the nested CG loops.
Suppose we write the arrays of link variables and a column vector \( v \) in the syntax of Fortran as

\[
\begin{align*}
  u(i, j, \mu, x), \\
  v(i, k, x),
\end{align*}
\]

where \( i \) and \( j \) are the color indices, \( \mu \) is the space-time direction, \( k \) is the spinor index, and \( x \) is the site index. Now the question is how to access the elements of these arrays in C routines. To resolve this problem, we define some data structures in C as follows.

```c
/* SU(3) matrix, (c01,c02) forms the complex number of u11, and 
   (c03,c04) of u21, etc. */
typedef struct {
  double c01, c02, c03, c04, c05, c06;
  double c07, c08, c09, c10, c11, c12;
  double c13, c14, c15, c16, c17, c18;
} su3_t;

/* there are 4 link variables at each site. */
typedef struct {
  su3_t mu1, mu2, mu3, mu4;
} ulink_t;

/* SU(3) vector, (c1,c2) forms the complex number of v1, 
   (c3,c4) of v2, and (c5,c6) of v3. */
typedef struct {
  double c1, c2, c3, c4, c5, c6;
} vector_t;

/* SU(3) Dirac spinor. */
typedef struct {
  vector_t s1, s2, s3, s4;
} spinor_t;
```

Then the correspondence can be easily established. For example, the elements \( u(3, 2, 1, x) \) and \( v(2, 4, x) \) can be accessed by C routines as (in the spinor space)

\[
\begin{pmatrix}
  r_1 \\
  r_2 \\
  r_3 \\
  r_4 
\end{pmatrix}
\]

\[
\begin{pmatrix}
  v_1 \\
  v_2 \\
  v_3 \\
  v_4 
\end{pmatrix}
\]

Then the multiplication of \( H_w \) to a column vector \(|v\rangle\) can be optimized by minimizing the number of multiplications involving the link variables. For example, the multiplication in \((-1 + \gamma_1)u|v\rangle\) can be written as (in the spinor space)

\[
\begin{pmatrix}
  r_1 \\
  r_2 \\
  r_3 \\
  r_4 
\end{pmatrix}
\]

\[
\begin{pmatrix}
  -u & 0 & 0 & u \\
  0 & -u & u & 0 \\
  0 & u & -u & 0 \\
  u & 0 & 0 & -u 
\end{pmatrix}
\]

\[
\begin{pmatrix}
  v_1 \\
  v_2 \\
  v_3 \\
  v_4 
\end{pmatrix}
\]

\[
\begin{pmatrix}
  u(v_4 - v_1) \\
  u(v_3 + v_2) \\
  -r_2 \\
  -r_1 
\end{pmatrix}
\]
where all indices are suppressed except the spinor indices. It is clear that the vectors $v_4 - v_1$ and $v_3 + v_2$ should be computed first, before they are multiplied by link variable $u$ ( generic symbol for $U_{\mu}/2$ ). For example, the operation $v_4 - v_1$ can be performed by the following macros with SSE2.

```c
#define mvpv(v1, v2)  
__asm__ __volatile__ ( 
   "movapd %0, %%xmm0 \n\t" 
   "movapd %1, %%xmm1 \n\t" 
   "movapd %2, %%xmm2 \n\t" 
   "subpd %3, %%xmm0 \n\t" 
   "subpd %4, %%xmm1 \n\t" 
   "subpd %5, %%xmm2" 
   :: 
   "m" ((v2).c1), 
   "m" ((v2).c3), 
   "m" ((v2).c5), 
   "m" ((v1).c1), 
   "m" ((v1).c3), 
   "m" ((v1).c5)
)
```

Similarly, we have

\[
(-I - \gamma_1)u^\dagger |v\rangle = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{pmatrix} = \begin{pmatrix} -u^\dagger(v_4 + v_1) \\ -u^\dagger(v_3 + v_2) \\ r_2 \\ r_1 \end{pmatrix},
\]

\[
(-I + \gamma_2)u |v\rangle = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{pmatrix} = \begin{pmatrix} -u(v_1 + iv_4) \\ -ir_3 \\ -u(v_3 + iv_2) \\ -ir_1 \end{pmatrix},
\]

\[
(-I - \gamma_2)u^\dagger |v\rangle = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{pmatrix} = \begin{pmatrix} -ir_4 \\ -u^\dagger(v_2 + iv_3) \\ -ir_2 \\ -u^\dagger(v_4 + iv_1) \end{pmatrix},
\]

\[
(-I + \gamma_3)u |v\rangle = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{pmatrix} = \begin{pmatrix} u(v_3 - v_1) \\ -u(v_2 + v_4) \\ -r_1 \\ r_2 \end{pmatrix},
\]

\[
(-I - \gamma_3)u^\dagger |v\rangle = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{pmatrix} = \begin{pmatrix} -u^\dagger(v_1 + v_3) \\ u^\dagger(v_4 - v_2) \\ -r_1 \\ r_2 \end{pmatrix},
\]
\[
(-\mathbb{I} + \gamma_4)u |v\rangle = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{pmatrix} = \begin{pmatrix} -ir_3 \\ -ir_4 \\ -u(v_3 + iv_1) \\ -u(v_4 + iv_2) \end{pmatrix},
\]

\[
(-\mathbb{I} - \gamma_4)u^\dagger |v\rangle = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{pmatrix} = \begin{pmatrix} -u^\dagger(v_1 + iv_3) \\ -u^\dagger(v_2 + iv_4) \\ -ir_1 \\ -ir_2 \end{pmatrix}.
\]

So the multiplications involving the link variables can be implemented as

```c
/* for each lattice size */
for (x=0; x<ldim; x++) {
    /* prefetch for the current multiplication */
    y = iup[x].mu1-1;
    _prefetch_su3(&u[x].mu1);
    _prefetch_spinor(&v[y]);

    /* prefetch for the next multiplication */
    z = idn[x].mu1-1;
    _prefetch_su3(&u[z].mu1);
    _prefetch_spinor(&v[z]);

    /* r1.s1 = u[x].mu1 * (v[y].s4 - v[y].s1) */
    mvpv(v[y].s1, v[y].s4);
    su3mul(r1.s1, u[x].mu1);

    /* r1.s2 = u[x].mu1 * (v[y].s3 - v[y].s2) */
    mvpv(v[y].s2, v[y].s3);
    su3mul(r1.s2, u[x].mu1);

    /* r1.s3 = -r1.s2 */
    mvset(r1.s3, r1.s2);

    /* r1.s4 = -r1.s1 */
    mvset(r1.s4, r1.s1);

    /* prefetch for the next multiplication */
    y = iup[x].mu2-1;
    _prefetch_su3(&u[x].mu2);
    _prefetch_spinor(&v[y]);

    /* r2.s1 = -(u[x].mu1)^\dagger * (v[y].s1 + v[y].s4) */
    mvmv(v[z].s1, v[z].s4);
    su3Hmul(r2.s1, u[z].mu1);

    /* r2.s2 = -(u[x].mu1)^\dagger * (v[y].s2 + v[y].s3) */
    mvmv(v[z].s2, v[z].s3);
    su3Hmul(r2.s2, u[z].mu1);

    /* r2.s3 = r2.s2 */
    pvset(r2.s3, r2.s2);

    /* r2.s4 = r2.s1 */
    pvset(r2.s4, r2.s1);
}
```
where $r_1$, $r_2$, \ldots, and $v[]$ are declared as the type \texttt{spinor\_t}, and $u[]$ is declared as the type \texttt{ulink\_t}. Note that prefetching has been inserted in order to attain the optimal performance. Finally, we have 8 vector segments $r_1$, \ldots, $r_8$, and a diagonal term. They are summed over to give the final result of $v[y]$

\[
\begin{align*}
  v[y].s_1 &= r_1.s_1 + r_2.s_1 + r_3.s_1 + r_4.s_1 + r_5.s_1 + r_6.s_1 + r_7.s_1 + r_8.s_1 + (4 - m_0) \ast v[x].s_1, \\
  v[y].s_2 &= r_1.s_2 + r_2.s_2 + r_3.s_2 + r_4.s_2 + r_5.s_2 + r_6.s_2 + r_7.s_2 + r_8.s_2 + (4 - m_0) \ast v[x].s_2, \\
  v[y].s_3 &= -(r_1.s_3 + r_2.s_3 + r_3.s_3 + r_4.s_3 + r_5.s_3 + r_6.s_3 + r_7.s_3 + r_8.s_3 + (4 - m_0) \ast v[x].s_3, \\
  v[y].s_4 &= -(r_1.s_4 + r_2.s_4 + r_3.s_4 + r_4.s_4 + r_5.s_4 + r_6.s_4 + r_7.s_4 + r_8.s_4 + (4 - m_0) \ast v[x].s_4.
\end{align*}
\]

Next we come to the question how to implement SSE2 codes for a $SU(3)$ matrix times a vector, the most crucial part in $H_w$ times $|v\rangle$. This problem has been solved by Lüscher [19], and his SSE2 codes is available in the public domain [20]. We found that Lüscher’s code is quite efficient, and have adopted it in our program. For completeness, we briefly outline Lüscher’s algorithm as follows.

Consider

\[
\begin{pmatrix}
  u_{11} & u_{12} & u_{13} \\
  u_{21} & u_{22} & u_{23} \\
  u_{31} & u_{32} & u_{33}
\end{pmatrix}
\times
\begin{pmatrix}
  y_1 \\
  y_2 \\
  y_3
\end{pmatrix}
=
\begin{pmatrix}
  r_1 \\
  r_2 \\
  r_3
\end{pmatrix}
\]

First, the elements $(y_1, y_2, y_3)$ of the vector $|y\rangle$ are copied to the registers %xmm0, %xmm1, and %xmm2, respectively. Then the real part of the $SU(3)$ matrix $\{u_{mn}\}$ is read sequentially, and is multiplied to $|y\rangle$ at %xmm0, %xmm1, and %xmm2, and the result is stored at %xmm3, %xmm4, and %xmm5,

\[
\begin{align*}
  %xmm0 &= (\text{Re}(y_1), \text{Im}(y_1)), \\
  %xmm1 &= (\text{Re}(y_2), \text{Im}(y_2)), \\
  %xmm2 &= (\text{Re}(y_3), \text{Im}(y_3)), \\
  %xmm3 &= (t_1, t_2), \\
  %xmm4 &= (t_3, t_4), \\
  %xmm5 &= (t_5, t_6),
\end{align*}
\]

where

\[
\begin{align*}
  t_1 &= \text{Re}(u_{11})\text{Re}(y_1) + \text{Re}(u_{12})\text{Re}(y_2) + \text{Re}(u_{13})\text{Re}(y_3), \\
  t_2 &= \text{Re}(u_{11})\text{Im}(y_1) + \text{Re}(u_{12})\text{Im}(y_2) + \text{Re}(u_{13})\text{Im}(y_3), \\
  t_3 &= \text{Re}(u_{21})\text{Re}(y_1) + \text{Re}(u_{22})\text{Re}(y_2) + \text{Re}(u_{23})\text{Re}(y_3), \\
  t_4 &= \text{Re}(u_{21})\text{Im}(y_1) + \text{Re}(u_{22})\text{Im}(y_2) + \text{Re}(u_{23})\text{Im}(y_3), \\
  t_5 &= \text{Re}(u_{31})\text{Re}(y_1) + \text{Re}(u_{32})\text{Re}(y_2) + \text{Re}(u_{33})\text{Re}(y_3), \\
  t_6 &= \text{Re}(u_{31})\text{Im}(y_1) + \text{Re}(u_{32})\text{Im}(y_2) + \text{Re}(u_{33})\text{Im}(y_3).
\end{align*}
\]
<table>
<thead>
<tr>
<th>Lattice Size</th>
<th>SSE2 off</th>
<th>SSE2 on</th>
<th>speed-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>$8^3 \times 24$</td>
<td>0.034</td>
<td>0.018</td>
<td>1.89</td>
</tr>
<tr>
<td>$10^3 \times 24$</td>
<td>0.065</td>
<td>0.036</td>
<td>1.81</td>
</tr>
<tr>
<td>$12^3 \times 24$</td>
<td>0.110</td>
<td>0.063</td>
<td>1.75</td>
</tr>
<tr>
<td>$16^3 \times 32$</td>
<td>0.328</td>
<td>0.183</td>
<td>1.79</td>
</tr>
</tbody>
</table>

Table 1: The execution time (in unit of second) for $H_w$ multiplying a column vector $Y$, with SSE2 turned on and off. The test is performed at a Pentium 4 (2 GHz) node.

Next, multiply the vector $y$ by $i = (0, 1)$, i.e.,

$$
\begin{align*}
%\text{xmm0} & \rightarrow (\text{Im}(y_1), \text{Re}(y_1)) \rightarrow (-\text{Im}(y_1), \text{Re}(y_1)), \\
%\text{xmm1} & \rightarrow (\text{Im}(y_2), \text{Re}(y_2)) \rightarrow (-\text{Im}(y_2), \text{Re}(y_2)), \\
%\text{xmm2} & \rightarrow (\text{Im}(y_3), \text{Re}(y_3)) \rightarrow (-\text{Im}(y_3), \text{Re}(y_3)),
\end{align*}
$$

which is implemented by the following SSE2 code

```c
static int sn3[4] ALIGN16 = {0x0,0x80000000,0x0,0x0};
#define su3mul(r, u) \
    ... \
    "xorpd %9, %xmm0 \n\t" \
    "xorpd %9, %xmm1 \n\t" \\
    "xorpd %9, %xmm2 \n\t" \\
    ... \\
    :: \\
    ... \\
    "m" (sn3[0]));
```

Then the imaginary part of $\{u_{mn}\}$ is read and multiplied to $iy$, and the final result is

$$
\begin{align*}
%\text{xmm3} & = (t_1 + s_1, t_2 + s_2), \\
%\text{xmm4} & = (t_3 + s_3, t_4 + s_4), \\
%\text{xmm5} & = (t_5 + s_5, t_6 + s_6),
\end{align*}
$$

where

$$
\begin{align*}
s_1 & = -\text{Im}(u_{11})\text{Im}(y_1) - \text{Im}(u_{12})\text{Im}(y_2) - \text{Im}(u_{13})\text{Im}(y_3), \\
s_2 & = +\text{Im}(u_{11})\text{Re}(y_1) + \text{Im}(u_{12})\text{Re}(y_2) + \text{Im}(u_{13})\text{Re}(y_3), \\
s_3 & = -\text{Im}(u_{21})\text{Im}(y_1) - \text{Im}(u_{22})\text{Im}(y_2) - \text{Im}(u_{23})\text{Im}(y_3), \\
s_4 & = +\text{Im}(u_{21})\text{Re}(y_1) + \text{Im}(u_{22})\text{Re}(y_2) + \text{Im}(u_{23})\text{Re}(y_3), \\
s_5 & = -\text{Im}(u_{31})\text{Im}(y_1) - \text{Im}(u_{32})\text{Im}(y_2) - \text{Im}(u_{33})\text{Im}(y_3), \\
s_6 & = +\text{Im}(u_{31})\text{Re}(y_1) + \text{Im}(u_{32})\text{Re}(y_2) + \text{Im}(u_{33})\text{Re}(y_3).
\end{align*}
$$
### Table 2: The execution time (in unit of second) for projecting 20 low-lying eigenmodes of $H_w^2$ using ARPACK, versus the number of Arnoldi vectors. The test is performed at a Pentium 4 (1.6 GHz) node, for a gauge configuration on the $8^3 \times 24$ lattice, at $\beta = 5.8$. Each eigenmode satisfies $\|(H_w^2 - \lambda^2)|x]\| < 10^{-13}$.

<table>
<thead>
<tr>
<th>Arnoldi vectors</th>
<th>Iterations</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>756</td>
<td>12923</td>
</tr>
<tr>
<td>50</td>
<td>160</td>
<td>4757</td>
</tr>
<tr>
<td>60</td>
<td>108</td>
<td>4730</td>
</tr>
<tr>
<td>70</td>
<td>82</td>
<td>4414</td>
</tr>
<tr>
<td>80</td>
<td>65</td>
<td>4131</td>
</tr>
<tr>
<td>90</td>
<td>55</td>
<td>4103</td>
</tr>
<tr>
<td>100</td>
<td>46</td>
<td>4100</td>
</tr>
<tr>
<td>120</td>
<td>37</td>
<td>4251</td>
</tr>
<tr>
<td>140</td>
<td>32</td>
<td>4869</td>
</tr>
<tr>
<td>160</td>
<td>26</td>
<td>5002</td>
</tr>
</tbody>
</table>

Table 5: Performance of the system

In this section, we measure the performance of our system by a number of tests pertaining to the computation of overlap Dirac quark propagators.

In Table 1, we list the execution time (in unit of second) for $H_w$ multiplying a column vector $Y$, for both cases with SSE2 turned on and off, and for several lattice sizes. The data shows that turning on SSE2 can speed up our program by a factor $\sim 1.8$.

In Table 2, we list the execution time (in unit of second) for projecting 20 low-lying eigenmodes of $H_w^2$ using ARPACK, versus the number of Arnoldi vectors. It is clear that there exists an optimal number of Arnoldi vectors for a projection, which of course depends on the gauge configuration. In Table 2, the optimal number is $\sim 100$, which amounts to $\sim 240$ Mbyte for the $8^3 \times 24$ lattice. However, for larger lattices such as $16^3 \times 32$, the optimal number may require more than one gigabyte of memory. In this case, the projection of eigenmodes is carried out at some nodes with 2 gigabyte of memory.

In Table 3, we measure the time used by disk I/O in our simple scheme of memory management for the nested CG loops, versus the number of bare quark masses. The test is performed at a Pentium 4 (2 GHz) node, for the $16^3 \times 32$ lattice, and with 16 projected eigenmodes. The disk I/O time is the difference of the total execution time between two cases of turning on and off of the memory management. It is remarkable that the percentage of disk I/O time is only 3% of the total execution time even for 16 bare quark masses, and with 16 projected eigenmodes. Evidently, for the $16^3 \times 32$ lattice, our simple scheme of memory management is more efficient and less expensive than any other options, e.g., parallel computing (with MPI) through a fast network switch.

In Table 4, we list the execution time (in unit of second) for a Pentium 4 (2 GHz) node to compute 12 columns of overlap Dirac quark propagators in a topologically nontrivial gauge background at $\beta = 5.8$ on the $8^3 \times 24$ lattice, versus the number of projected low-lying eigenmodes. Other parameters for the test are: the degree of Zolotarev rational polynomial
Table 3: The percentage of time spent in memory management (disk I/O) versus the number of bare quark masses ($N_m$). The test is performed at a Pentium 4 (2 GHz) node, for the $16^3 \times 32$ lattice, and with 16 projected eigenmodes. The time (in unit of second) shown here is only for completing one outer CG iteration for one column of $D^{-1}$.

<table>
<thead>
<tr>
<th>$N_m$</th>
<th>1</th>
<th>8</th>
<th>16</th>
</tr>
</thead>
<tbody>
<tr>
<td>CG time</td>
<td>491.9</td>
<td>494.8</td>
<td>497.1</td>
</tr>
<tr>
<td>disk I/O time</td>
<td>7.6</td>
<td>8.9</td>
<td>14.3</td>
</tr>
<tr>
<td>Total time</td>
<td>499.5</td>
<td>503.7</td>
<td>511.4</td>
</tr>
<tr>
<td>disk I/O (%)</td>
<td>1.5%</td>
<td>1.8%</td>
<td>2.9%</td>
</tr>
</tbody>
</table>

is $n = 16$; the number of bare quark masses is $N_m = 12$; each projected eigenmode satisfies $\| (H_w^2 - \lambda^2) | x \rangle \| < 10^{-13}$, and the stopping criterion for inner and outer CG loops is $\epsilon = 10^{-11}$. The execution time is decomposed into three parts: (i) the projections of high and low-lying eigenmodes$^4$; (ii) computing 12 columns of $(DD^\dagger)^{-1}$ via the nested CG loops; and (iii) computing $D^\dagger$ and multiplying it to $(DD^\dagger)^{-1}$. The total time is listed in the last column of the table. For completeness, we also list $\lambda_{\text{max}}$ and $\lambda_{\text{min}}$ of $|\bar{H}_w|$ (after the projections), the total numbers of iterations of the outer CG loop and average iterations of the inner CG loop, as well as the precision of exact chiral symmetry in terms of $\sigma$ (13). Evidently, the time for projecting out the high and low-lying eigenmodes is only a very small fraction of the total execution time for computing 12 columns of quark propagators. However, the projections have very significant impacts on the total execution time since it yields the speed-up by a factor of 2.44, as comparing the first row (no projections) with the last row (projections of 40 low-lying eigenmodes). Moreover, with projections, the exact chiral symmetry can be easily preserved to a very high precision ($\sigma < 10^{-13}$). This suggests that one should project as many low-lying eigenmodes as possible, before executing the nested CG loops. In general, we suspect that the optimal number of projections depends on the projection algorithm, the amount of memory of the system, as well as the gauge configuration.

In Table 5, we measure the precision of exact chiral symmetry $\sigma$ (13) versus the degree $(n)$ of Zolotarev optimal rational polynomial. The values of $\sigma$ listed in the second column of Table 5 are the maxima in the nested CG loops. The execution time and the iterations of the nested CG loops are also listed. Evidently, the precision of exact chiral symmetry $\sigma$ is quite different from the stopping criterion $\epsilon = 10^{-11}$ for inner and outer CG loops, since $\sigma$ can be much bigger or smaller than $\epsilon$, as shown in Table 5, as well as in Tables 4 and 6. It is clear that the necessary condition for preserving exact chiral symmetry to a very high precision is to use a higher degree $(n)$ Zolotarev rational polynomial for $(H_w^2)^{-1/2}$. In Ref. [13], tables are provided for looking up which degree $n$ is required to attain one’s desired accuracy in preserving the exact chiral symmetry on the lattice, versus the parameter $b = \lambda_{\text{max}}^2 / \lambda_{\text{min}}^2$ of a given gauge configuration.

In Table 6, we list the execution time (in unit of second) of a Pentium 4 (2 GHz) node to compute 12 columns of overlap Dirac quark propagators, versus the size of the lattice. The parameters for the test are: the degree of Zolotarev rational polynomial is $n = 16$, the

$^4$Note that the projection time listed in the 4-th column of Table 4 includes 167 seconds for projecting 4 highest eigenmodes of $H_w$. 

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Table 4: The execution time for a Pentium 4 (2 GHz) node to compute 12 columns of overlap Dirac quark propagators, versus the number of projected low-lying eigenmodes. The parameters for the test are: the lattice size is $8^3 \times 24$; $\beta = 5.8$; the degree of Zolotarev rational polynomial is $n = 16$; the number of bare quark masses is $N_m = 12$ and $ma \geq 0.06$; each projected eigenmode satisfies $\| (H_w^2 - \lambda^2) |x\rangle \| < 10^{-13}$; and the stopping criterion for inner and outer CG loops is $\epsilon = 10^{-11}$.

<table>
<thead>
<tr>
<th>#</th>
<th>time</th>
<th>$\lambda_{\min}$</th>
<th>$\lambda_{\max}$</th>
<th>inner CG ave. iters.</th>
<th>outer CG tot. iters.</th>
<th>$\chi$ sym. $\sigma(\text{max.})$</th>
<th>CG time</th>
<th>$D^{\dagger}$ mult. time</th>
<th>Total time</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0.017</td>
<td>6.207</td>
<td>965</td>
<td>1282</td>
<td>$4.5 \times 10^{-10}$</td>
<td>137221</td>
<td>15070</td>
<td>152291</td>
</tr>
<tr>
<td>8</td>
<td>1573</td>
<td>0.138</td>
<td>6.207</td>
<td>552</td>
<td>1282</td>
<td>$5.2 \times 10^{-14}$</td>
<td>70908</td>
<td>7828</td>
<td>80309</td>
</tr>
<tr>
<td>16</td>
<td>2753</td>
<td>0.165</td>
<td>6.207</td>
<td>475</td>
<td>1282</td>
<td>$5.7 \times 10^{-14}$</td>
<td>61543</td>
<td>6803</td>
<td>71099</td>
</tr>
<tr>
<td>24</td>
<td>3703</td>
<td>0.178</td>
<td>6.207</td>
<td>443</td>
<td>1282</td>
<td>$4.3 \times 10^{-14}$</td>
<td>57792</td>
<td>6374</td>
<td>67869</td>
</tr>
<tr>
<td>32</td>
<td>4725</td>
<td>0.198</td>
<td>6.207</td>
<td>403</td>
<td>1282</td>
<td>$5.3 \times 10^{-14}$</td>
<td>52961</td>
<td>5864</td>
<td>63550</td>
</tr>
<tr>
<td>40</td>
<td>6524</td>
<td>0.211</td>
<td>6.207</td>
<td>378</td>
<td>1282</td>
<td>$6.0 \times 10^{-14}$</td>
<td>50301</td>
<td>5581</td>
<td>62409</td>
</tr>
</tbody>
</table>

Table 5: The precision of exact chiral symmetry $\sigma$ versus the degree ($n$) of the Zolotarev rational polynomial. The test is performed at a Pentium 4 (2 GHz) node, with the parameters: lattice size=$16^3 \times 32$; $\beta = 6.0$; the number of bare quark masses is $N_m = 16$; the number of projected eigenmodes is $k = 20$; each projected eigenmode satisfies $\|(H_w^2 - \lambda^2) |x\rangle \| < 10^{-13}$; $b = \lambda_{\max}^2/\lambda_{\min}^2 = 1086$; and the stopping criterion for the CG loops is $\epsilon = 10^{-11}$.

<table>
<thead>
<tr>
<th>Zolo. degree</th>
<th>$\chi$ sym. $\sigma(\text{max.})$</th>
<th>CG iters. inner</th>
<th>CG iters. outer</th>
<th>CG time</th>
<th>$D^{\dagger}$ mult. time</th>
<th>Total time</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>$1.7 \times 10^{-4}$</td>
<td>367</td>
<td>286</td>
<td>82393</td>
<td>4493</td>
<td>86885</td>
</tr>
<tr>
<td>8</td>
<td>$1.5 \times 10^{-8}$</td>
<td>402</td>
<td>288</td>
<td>111247</td>
<td>6003</td>
<td>117250</td>
</tr>
<tr>
<td>10</td>
<td>$2.9 \times 10^{-10}$</td>
<td>408</td>
<td>288</td>
<td>120940</td>
<td>6520</td>
<td>127460</td>
</tr>
<tr>
<td>12</td>
<td>$6.4 \times 10^{-12}$</td>
<td>411</td>
<td>288</td>
<td>129188</td>
<td>6962</td>
<td>136150</td>
</tr>
<tr>
<td>16</td>
<td>$1.4 \times 10^{-13}$</td>
<td>414</td>
<td>288</td>
<td>148654</td>
<td>8006</td>
<td>156660</td>
</tr>
</tbody>
</table>

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number of bare quark masses is $N_m = 16$ and $m a \geq 0.02$, each projected eigenmode satisfies $\| (H_w^2 - \lambda^2) | x \| < 10^{-13}$, and the stopping criterion for the inner and the outer CG loops is $\epsilon = 10^{-11}$. From the last entry of the last row, we can estimate that a Pentium 4 (2 GHz) node takes about 24 days to complete 12 columns of overlap Dirac quark propagators (for 16 bare quark masses) for one gauge configuration at $\beta = 6.0$ on the $16^3 \times 32$ lattice. In other words, if we have 12 nodes and let each one of them work on one column of $D^{-1}$, then we can complete the overlap Dirac quark propagators for one gauge configuration in two days. Since our system consists of 30 nodes, in which 12 nodes are Pentium 4 (2.0 GHz), and 18 nodes are Pentium 4 (1.6 GHz), so we can compute overlap Dirac quark propagators at a rate more than two gauge configurations per two days.

6 Conclusions

In this paper, we have outlined the essential features of a Linux PC cluster which is now being developed at National Taiwan University, and discussed how to optimize its hardware and software for lattice QCD with overlap Dirac quarks.

With Zolotarev optimal rational approximation to $(H_w^2)^{-1/2}$, projections of high and low-lying eigenmodes of $H_w^2$, the multi-mass CG algorithm, the SSE2 acceleration, and our simple scheme of memory management, we are able to compute overlap Dirac quark propagators of 16 bare quark masses on the $16^3 \times 32$ lattice, with the precision of quark propagators up to $10^{-11}$ and the precision of exact chiral symmetry up to $10^{-12}$, at the rate of one gauge configuration ($\beta = 6.0$) per day, with our present system of 30 nodes. This demonstrates that an optimized Linux PC cluster can be a viable computational system to extract physical quantities from lattice QCD with overlap Dirac quarks [9, 21, 22].

The speed of our system is higher than 30 Gflops, and the total cost of the hardware is less than US$30,000. This amounts to price/performance better than $1.0/Mflops for 64-bit (double precision) computations with overlap Dirac quarks. The basic idea of optimization is to let each node work independently on one of the 12 columns of the quark propagators (for a set of bare quark masses), and also use the hard disk as the virtual memory for the vectors in the outer CG loop, while the CPU is working on the inner CG loop. Our simple scheme of memory management for the nested CG loops may also be useful to other systems.

In future, we will add more nodes to our system, and will also work on larger lattices, say $24^3 \times 48$. Then one Gbyte memory at each node is not sufficient to accommodate all relevant vectors in the inner CG loop, even for 12 Zolotarev terms. However, there are several ways to circumvent this problem. First, our memory management scheme is quite versatile, which is more than just for swapping the vectors at the interface of inner and outer CG loops. In fact, it can handle any number of Zolotarev terms for any lattice size, and can automatically minimize disk I/O at any step of the nested CG loops, according to the amount of physical memory of a node. As long as the percentage of the disk I/O time is less than 30%, it is still a better option than distributing the nested CG loops across the nodes and performing parallel computations (with MPI) through a fast network switch, since the communication overheads is expected to be more than 30% of the total time, especially for a system of 100 nodes or more. Secondly, we can increase the amount of memory at each node, which depends on the specification of the motherboard as well as the price and the capacity of the memory modules. Finally, we can also exploit algorithms [23] which only use 4 vectors rather than $2n + 3$ vectors.
Table 6: The execution time (in unit of second) of a Pentium 4 (2 GHz) node to compute 12 columns of overlap Dirac quark propagators, versus the size of the lattice. The parameters for the test are: the degree of Zolotarev rational polynomial is $n = 16$, the number of bare quark masses is $N_m = 16$ and $ma \geq 0.02$, the precision of each projected eigenmode satisfies $\| (H_w^2 - \lambda^2) |x_0 > \| < 10^{-13}$, and the stopping criterion for inner and outer CG loops is $\epsilon = 10^{-11}$.
for the inner CG loop, at the cost of executing two passes for each inner CG iteration but the slow-down is less than by a factor of two, or the Lanczos algorithm as described in Ref. [24]. Now it is clear that a Linux PC cluster is a viable platform to tackle lattice QCD with overlap Dirac quarks even for a large lattice (e.g., $32^3 \times 64$), though more studies are needed before one reaches an optimal design for larger ones.

Acknowledgement

This work was supported in part by the National Science Council, ROC, under the grant number NSC90-2112-M002-021.
References


