A note on Neuberger’s double pass algorithm

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Abstract

We analyze Neuberger’s double pass algorithm for the matrix-vector multiplication $R(H) \cdot Y$ (where $R(H)$ is $(n - 1, n)$-th degree rational polynomial of positive definite operator $H$), and show that the number of floating point operations is independent of the degree $n$, provided that the number of sites is much larger than the number of iterations in the conjugate gradient. This implies that the matrix-vector product $(H)^{-1/2}Y \simeq R(n-1,n)(H) \cdot Y$ can be approximated to very high precision with sufficiently large $n$, without noticeably extra costs. Further, we show that there exists a threshold $n_T$ such that the double pass is faster than the single pass for $n > n_T$, where $n_T \simeq 12 - 25$ for most platforms.

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1 Introduction

In 1998, Neuberger proposed the nested conjugate gradient \[1\] for solving the propagator of the overlap-Dirac operator \[2\]

\[
D = m_0 \left( 1 + \gamma_5 \frac{H_w}{\sqrt{H_w^2}} \right),
\]
with the sign function \(\text{sgn}(H_w) \equiv H_w(H_w^2)^{-1/2}\) approximated by the polar approximation

\[
S(H_w) = \frac{H_w}{n} \sum_{l=1}^{n} b_l H_w^2 + d_l = H_w R_{(n-1,n)}(H_w^2),
\]

where \(H_w = \gamma_5 D_w\), and \(D_w\) is the standard Wilson-Dirac operator plus a negative parameter \(-m_0\) \((0 < m_0 < 2)\), and the coefficients \(b_l\) and \(d_l\) are:

\[
b_l = \sec^2 \left[ \frac{\pi}{2n} \left( l - \frac{1}{2} \right) \right], \quad d_l = \tan^2 \left[ \frac{\pi}{2n} \left( l - \frac{1}{2} \right) \right].
\]

In principle, any column vector of \(D^{-1} = D^\dagger (DD^\dagger)^{-1}\) can be obtained by solving the system

\[
DD^\dagger Y = n_0^2 [2 + \gamma_5 S(H_w) + S(H_w)\gamma_5] Y = \mathbb{I}
\]

with conjugate gradient, provided that the matrix-vector product \(S(H_w)Y\) can be carried out. Writing

\[
S(H_w)Y = \frac{H_w}{n} \sum_{l=1}^{n} b_l Z^{(l)},
\]

one can obtain \(\{Z^{(l)}\}\) by solving the system

\[
(H_w^2 + d_l) Z^{(l)} = Y
\]

with multi-shift conjugate gradient \[3\] \[4\]. In other words, each (outer) CG iteration in \[3\] contains a complete (inner) CG loop \[5\], i.e., nested conjugate gradient.

Evidently, the overhead for the nested conjugate gradient is the execution time for the inner conjugate gradient loop \[5\] as well as the memory space it requires, i.e., \((2n + 3)\) large vectors, each of \(12N_{\text{site}}\) double complex numbers, where \(N_{\text{site}}\) is the number of sites, and \(12 = 3\) (color) \(\times 4\) (Dirac) is the degrees of freedom at each site for QCD. The memory storage becomes prohibitive for large lattices since \(n\) is often required to be larger than 16 in order to achieve a reliable approximation for the sign function. To minimize the memory storage...
for \( \{P^{(l)}, Z^{(l)}\} \), Neuberger [5] observed that one only needs the linear combination \( \sum_{i=1}^{n} b_i Z^{(l)} \) rather than each \( Z^{(l)} \) individually. Since \( Z^{(l)}_i \) and its conjugate vector \( P^{(l)}_i \) at the \( i \)-th iteration of the inner CG are linear combinations of their preceedents \( \{P^{(l)}_j, Z^{(l)}_j, j = 0, \cdots, i-1\} \) in the iteration process, thus it is possible to obtain their updating coefficients \( \{\alpha^{(l)}_i, \beta^{(l)}_i\} \) in the first pass, and then use them to update the sum \( \sum_{i=1}^{n} b_i Z^{(l)} \) successively in the second pass, with memory storage of only 5 vectors, independent of the degree \( n \) of the rational polynomial \( R^{(n-1,n)} \).

At first sight, the double pass algorithm seems to be slower than the single pass algorithm. However, in the test run (with SU(2) gauge field on the \( 8^3 \) lattice), Neuberger found that the double pass actually ran faster by 30\% than the single pass, and remarked that the speedup most likely reflects the cache usage in the testing platform, the SGI O2000 (with four processors, each with 4MB cache memory).

In this paper, we analyze the number of floating point operations \( (F_2) \) for the double pass algorithm, and show that it is independent of the degree \( n \) of \( R^{(n-1,n)} \), provided that the number of lattice sites \( (N_{\text{site}}) \) is much larger than the number of iterations \( (L_i) \) of the CG loop. The last condition is amply satisfied even for a small lattice (e.g., \( N_{\text{site}} = 8^3 \times 24 = 12288 \)), since \( L_i \) is usually less than 1000 (after the low-lying eigenmodes of \( H_w^2 \) are projected out). On the other hand, the number of floating point operations \( (F_1) \) for the single pass is a linearly increasing function of \( n \). It follows that there exists a threshold \( n_F \) such that \( F_2 \leq F_1 \) for \( n \geq n_F \), where the value of \( n_F \) depends on the implementation of the algorithms (\( n_F \simeq 59 \) for our codes). Corresponding to the number of floating point operations, we also obtain the formulas for the CPU times \( (T_1 \text{ and } T_2) \) for the single and the double pass algorithms. Further, we show that there exists a threshold \( n_T \) such that the double pass is faster than the single pass\(^1\) for \( n > n_T \), where \( n_T \simeq 12 - 25 \) (for most platforms), which is quite smaller than the threshold \( n_F \simeq 59 \) for the number of floating point operations. By timing the speed of each subroutine, we can account for the extra slow down in the single pass algorithm, which is unlikely to be eliminated, due to the memory bandwidth, a generic weakness of any computational system. Thus, in general (for most vector or superscalar machines), one may find that the double pass is faster than the single pass, for \( n > n_T \simeq 12 - 25 \). This explains why in Neuberger’s test run, even at \( n = 32 \), the double pass is already faster than the single pass by 30\%. In fact, we find that DEC alpha XP1000 and IBM SP2 SMP also have 30\% speedup at \( n = 32 \) (see Table 4), which agrees with the theoretical estimate (32) using the CPU time formulas (27)-(28).

Nevertheless, the most interesting result is that the speed of the double pass

\(^1\)In this paper, we only consider the (faster) single pass algorithm in which the vectors \( P^{(l)} \) and \( Z^{(l)} \) \((l = 2, \cdots, n)\) are not updated after \( Z^{(l)} \) converges.
algorithm is almost independent of the degree \( n \). This implies that the matrix-vector product \( (H_w^2)^{-1/2}Y \approx R^{(n-1,n)}(H_w^2)Y \) can be approximated to very high precision with sufficiently large \( n \), without noticeably extra costs.

The outline of this paper is as follows. In section 2, we outline the single and double pass algorithms for the iteration of the (inner) CG loop (5), and analyze their major differences. In section 3, we estimate the number of (double precision) floating point operations as well as the CPU time for the single and double pass algorithms respectively, and show that there exists a threshold \( n_T \) such that the double pass is faster than the single pass for \( n > n_T \). In section 4, we perform some tests. In section 5, we conclude with some remarks.

2 The single and double pass algorithms

In the section, we outline the single and the double pass algorithms for the inner CG loop (5), and point out their major differences.

For the single pass algorithm, with the input vector \( Y \), we initialize the vector variables \( \{Z^{(l)}, P^{(l)}\} \), \( R, A, B \) and the scalar variables \( \alpha, \beta, \{\gamma^{(l)}\} \) as

\[
Z_0^{(l)} = 0, \quad P_0^{(l)} = Y, \quad l = 1, \ldots, n
\]
\[
R_0 = Y,
\]
\[
\alpha_{-1} = 1,
\]
\[
\beta_0 = 0,
\]
\[
\gamma_{-1}^{(l)} = \gamma_0^{(l)} = 1, \quad l = 1, \ldots, n
\]

Then we iterate \((j = 0, 1, \ldots)\) according to:

\[
A_j = H_wP_j^{(1)}
\]
\[
B_j = H_wA_j + d_1P_j^{(1)} = (H_w^2 + d_1)P_j^{(1)}
\]
\[
\alpha_j = \frac{\langle R_j|R_j \rangle}{\langle P_j^{(1)}|B_j \rangle}
\]
\[
R_{j+1} = R_j - \alpha_jB_j
\]
\[
\beta_{j+1} = \frac{\langle R_{j+1}|R_{j+1} \rangle}{\langle R_j|R_j \rangle}
\]
\[
P_{j+1}^{(1)} = R_{j+1} + \beta_{j+1}P_j^{(1)}
\]
\[
Z_{j+1}^{(1)} = Z_j^{(1)} + \alpha_jP_j^{(1)}
\]

Together with the following updates for \( l = 2, \ldots, n \):

\[
\gamma_{j+1}^{(l)} = \frac{\gamma_{j}^{(l)} \gamma_{j-1}^{(l)} \alpha_{j-1}}{\alpha_j \beta_j (\gamma_{j-1}^{(l)} - \gamma_j^{(l)}) + \gamma_{j-1}^{(l)} \alpha_{j-1} (1 + \alpha_j (d_l - d_1))}
\]
\[ P_{j+1}^{(l)} = \gamma_{j+1}^{(l)} R_{j+1} + \beta_{j+1} \left( \frac{\gamma_{j+1}^{(l)}}{\gamma_{j}^{(l)}} \right)^2 P_{j}^{(l)} \]  
(14)

\[ Z_{j+1}^{(l)} = Z_{j}^{(l)} + \alpha_{j} \frac{\gamma_{j+1}^{(l)}}{\gamma_{j}^{(l)}} P_{j}^{(l)} . \]  
(15)

The loop terminates at the \( i \)-th iteration if \( \sqrt{\langle R_{i+1} | R_{i+1} \rangle / \langle Y | Y \rangle} \) is less than the tolerance (tol).

Since we are only interested in the linear combination \( \sum_{l=1}^{n} b_{l} Z_{i+1}^{(l)} \), in which each \( Z_{i+1}^{(l)} \) can be expressed in terms of \( \{ R_{j}, j = 0, \cdots, i \} \), thus we can write

\[ \sum_{l=1}^{n} b_{l} Z_{i+1}^{(l)} = \sum_{j=0}^{i} c_{j} R_{j} \]  
(16)

where \( c_{j} \) can be derived as [5]

\[ c_{j} = \sum_{m=0}^{i-j} \alpha_{j+m} \delta_{m} \left[ b_{1} + \sum_{l=2}^{n} b_{l} \gamma_{m+j+1}^{(l)} / \gamma_{j}^{(l)} \right] , \]  
(17)

with

\[ \delta_{m} = \begin{cases} \prod_{k=1}^{m} \beta_{j+k} , & \text{for } m > 0 , \\ 1 , & \text{for } m = 0 . \end{cases} \]  
(18)

Therefore, the r.h.s. of (16) can be evaluated with the CG loop (6)-(11), requiring only the storage of 5 large vectors \((A, B, R, P^{(1)}, T = \sum c_{j} R_{j})\), provided that the coefficients \( \{ c_{j}, j = 0, \cdots, i \} \) are known. However, from (17), the determination of \( c_{j} \) at any \( j \)-th iteration requires some values of \( \{ \alpha \} \), \( \{ \beta \} \) and \( \{ \gamma \} \) which can only be obtained in later iterations. Thus we have to run the first pass, i.e., the CG loop (6)- (11), to obtain all coefficients of \( \{ \alpha \} \), \( \{ \beta \} \) up to the convergence point \( i \), and then compute all \( \{ c_{j}, j = 0, \cdots, i \} \) according to (17) and (13). Finally, we run the second pass, i.e., going through (6), (7), (9), (11), and adding \( c_{j} R_{j} \) to the r.h.s. of (16), successively from \( j = 0 \) to the convergence point \( i \).

Evidently, all operations in (6)-(12) and (14)-(15) are proportional to the number of lattice sites \( N_{\text{site}} \) times the number of iterations \( L_{i} \). On the other hand, the computations of the coefficients \( \{ \gamma \} \) (13) and \( \{ c_{j} \} \) (17) do not depend on \( N_{\text{site}} \), but only on \( L_{i} \) (up to a small term proportional to \( L_{i}^{3} \)). Thus, for \( N_{\text{site}} \gg L_{i} \), we can neglect the computation of \( \{ c_{j} \} \) (17), and focus on the major difference between the single pass and the double pass, namely, the number of operations in (14)-(15), which is proportional to \((n-1)N_{\text{site}}L_{i}\), versus the number of operations in (6), (7), (9), (11) plus the vector update on the r.h.s. of (16), which is proportional to \( N_{site}L_{i} \). Obviously, the number...
of floating-point operations in the single pass is a linearly increasing function of \( n \), while that of the double pass is independent of \( n \), thus it follows that the double pass must be faster than the single pass for sufficiently large \( n \).

In the next section, we estimate the number of floating point operations as well as the CPU time, for the single pass and the double pass respectively. Even though our countings are based on our codes, they serve to illustrate the general features of the single and the double pass algorithms, which are valid for any software implementations and/or machines.

3 The CPU time and the number of floating point operations

For our codes, the number of floating point operations for the single pass is

\[
F_1 = N_{\text{site}} L_i [3552 + 120(n - 1)p] + N_{\text{site}} (288n_{ev} + 48n + 1776),
\]

while for the double pass is

\[
F_2 = 6888 N_{\text{site}} L_i + N_{\text{site}} (288n_{ev} - 1656) + \left[ \frac{L_i^3}{6} + L_i^2 (2n - 1) + L_i \left( 13n - \frac{73}{6} \right) - 7n + 7 \right] q
\]

where \( N_{\text{site}} \) is the number of sites of the lattice, \( L_i \) is the number of iterations of the CG loop, \( n_{ev} \) is the number of projected eigenmodes of \( H_w^2 \), and \( n \) is the degree of the rational polynomial \( R^{(n-1,n)} \). In the single pass, Eq. (19), \( (n - 1)p \) is the effective number of the \( (n - 1) \) updates in (14)-(15), since \( P^{(l)} \) and \( Z^{(l)} \) are not updated after \( Z^{(l)} \) converges. The value of \( p \) depends on the convergence criteria as well as the rational polynomial \( R^{(n-1,n)} \) and its argument. Similarly, in the double pass, the sum in (17) only includes the terms which have not yet converged at the iteration \( j \), and the reduction in the number of floating point operations can be taken into account by the factor \( q \) in (20). (The value of \( q \) is about 0.95 for convergence up to the zero in the IEEE double precision representation).

Taking into account of different speeds of various floating point operations, we estimate the CPU time for the single pass and the double pass as follows.

\[
T_1 = N_{\text{site}} L_i [192t_b + 72t_c + 3288t_d + (48t_b + 72t_a)(n - 1)p] + N_{\text{site}} (288n_{ev}t_c + 48nt_b + 24t_a + 108t_c + 1644t_d)
\]

\[
T_2 = N_{\text{site}} L_i (240t_b + 72t_c + 6576t_d) + N_{\text{site}} (288n_{ev}t_c + 24t_a - 144t_b + 108t_c - 1644t_d) + q \left[ \frac{L_i^3}{6} + L_i^2 (2n - 1) + L_i \left( 13n - \frac{73}{6} \right) - 7n + 7 \right] t_f
\]
where $t_a, t_b, t_c$ and $t_d$ denote the average CPU time per floating-point operation (FPO) for the four different kinds of vector operations (a)-(d) listed in Table 1 respectively, $t_e$ the average CPU time per FPO for constructing the complementary vector from the projected eigenmodes of $H_w$, and $t_f$ the time for computing the coefficients (17) in the double pass. Note that setting $t_a = t_b = t_c = t_d = t = t_e = t_f = 1$ in (21) and (22) reproduce (19) and (20) respectively.

It should be emphasized that the numerical values of the constants and coefficients in (19)-(22) may vary slightly from one implementation to another, however, the number of different terms and their functional dependences on the variables ($N_{site}$, $L_i$, $n$, $n_{ev}$, $p$, $q$, $t_a$, $t_b$, $t_c$, $t_d$, $t_e$, and $t_f$) should be the same for any codes of the single and double pass algorithms.

For the double pass, it is clear that the first term on the r.h.s. of Eq. (20) is the most significant part, since the number of lattice site ($N_{site}$) is usually much larger than the number of iterations ($L_i$) of the CG loop such that the second and the third terms on the r.h.s. of (20) can be neglected. For example, $N_{site} = 8^3 \times 24$, $L_i = 1000$, $n = 16$, $n_{ev} = 32$ and $q = 0.95$, then the first term is $6888 N_{site} L_i \approx 8.5 \times 10^{10}$, while the sum of the second and the third terms only gives $\sim 2.8 \times 10^8$. Thus we can single out the most significant part of $F_2$,

$$F_2 \approx 6888 N_{site} L_i ,$$

which comes from the first pass (6)-(11) and the second pass (6), (7), (9), (11) plus the vector update on the r.h.s. of (16). Similarly, for the single pass, the most significant part of $F_1$ is the first term on the r.h.s. of (19)

$$F_1 \approx N_{site} L_i [3552 + 120(n - 1)p] ,$$

which comes from the operations in (6)-(12), and (14)-(15).

Evidently, from (24) and (23), $F_1$ is a linearly increasing function of $n$ while $F_2$ is independent of $n$. Thus it follows that there exists a threshold $n_F$ such that $F_2 < F_1$ for $n > n_F$. From (24) and (23), we obtain the threshold $n_F$,

$$n_F = 1 + \frac{139}{5p} ,$$

where the value of $p$ depends on the convergence criterion for removing $\{P^{(l)}, Z^{(l)}\}$ from the updating list, as well as the rational polynomial $R(n-1,n)$ and its argument. For our codes and the tests in the next section, $p \approx 0.48$, thus we have

$$n_F \approx 59 .$$

Assuming $N_{site} \gg L_i$, we obtain the most significant parts of the CPU times (21)-(22) as

$$T_1 \approx N_{site} L_i [192t_b + 72t_c + 3288t_d + (48t_b + 72t_a)(n - 1)p] ,$$

$$T_2 \approx N_{site} L_i (240t_b + 72t_c + 6576t_d) .$$
Obviously, from (27) and (28), there exists a threshold

\[ n_T = 1 + \frac{2t_b + 137t_d}{(2t_b + 3t_a)p} \]  

(29)

such that \( T_2 < T_1 \) (the double pass is faster than the single pass) for \( n > n_T \).

Even though the countings in (21) and (22) are based on our codes (for \( R^{(n-1,n)} \) with argument \( H_w^2 \)), the essential features of (21) and (22) should be common to all implementations of the single and the double pass algorithms. In other words, the numerical coefficients in (27) and (28) may change from one implementation to another, however, \textit{the existence of a threshold \( n_T \) must hold for any implementation.}

Now it is interesting to compare \( n_T \) with \( n_F \). From (25) and (29), one immediately sees that \( n_T < n_F \) if

\[ 19t_d < 11t_a + 7t_b \]  

(30)

is satisfied\(^2\).

In practice, it turns out that \( t_a/t_d > 2 \) and \( t_b/t_d > 3 \) for most systems (Tables 1-2). Thus, \( n_T \approx 12 - 25 \), which is quite smaller than \( n_F \approx 59 \).

The speedup of the double pass with respect to the single pass (for \( n > n_T \)) can be defined as

\[ S = \frac{T_1 - T_2}{T_2} \]  

(31)

which is estimated to be

\[ S \approx \frac{(3t_a + 2t_b)p}{10t_b + 3t_c + 274t_d}(n - n_T) \]  

(32)

where Eqs. (27)-(29) have been used.

In Table 1, we list our measurements of \( t_a, t_b, t_c \) and \( t_d \) for four different hardware configurations of Pentium 4, i.e., two different Rambuses of faster/slower (PC1066/PC800) speed, and with/without SSE2 (the vector processing unit of Pentium 4) codes.

Substituting the values of \( t_a, t_b \) and \( t_d \) into (29), we obtain the theoretical estimates for the threshold \( n_T \),

\[ n_T \approx \begin{cases} 12, & \text{Pentium 4, PC800, with SSE2,} \\ 22, & \text{Pentium 4, PC800,} \\ 13, & \text{Pentium 4, PC1066, with SSE2,} \\ 25, & \text{Pentium 4, PC1066,} \end{cases} \]  

(33)

where \( p \approx 0.48 \) has been used.

\(^2\)Note that the inequality (30) is more restrictive than \( 685t_d < 417t_a + 268t_b \).
Table 1: The average CPU time (in unit of nano-second) per floating point operation (FPO) for 4 different kinds of matrix-vector operations in the single and double pass algorithms. The CPU is Pentium 4 (2.53 GHz), with one Gbyte Rambus (PC800 or PC1066).

| Operation | # of FPO | CPU time(ns) per FPO |
|-----------|----------|----------------------|
|           |          | PC800 | PC1066 |
|           |          | SSE2 on | off | SSE2 on | off |
| (a) | $|A\rangle = c_1|A\rangle + c_2|B\rangle$ | $72 \times N_{site}$ | 3.720 | 3.721 | 2.977 | 3.016 |
| (b) | $|V\rangle = |A\rangle + c|B\rangle$ | $48 \times N_{site}$ | 5.521 | 5.522 | 4.330 | 4.429 |
| (c) | $\alpha = \langle V|V \rangle$ | $36 \times N_{site}$ | 4.249 | 4.251 | 3.312 | 3.340 |
| (d) | $|A\rangle = H_w|B\rangle$ | $1644 \times N_{site}$ | 0.764 | 1.535 | 0.686 | 1.440 |

Note that for each hardware configuration in Table 1, the average CPU time per FPO of the simple vector operations (a)-(c) is much longer than that of (d), Wilson matrix times vector. A simplified explanation\(^3\) is as follows. Since all these four vector operations involve long vectors, the CPU and its cache cannot hold all data at once. Thus it is necessary to transfer the data from/to the memory successively, every time after the CPU completes its operations on a portion of the vectors. However, for any system, the memory bandwidth is limited. Thus, there is a time interval between consecutive sets of data transferring to/from the CPU. Therefore, if the CPU finishes a computation before the next set of data is ready, then it would waste its cycles in idling. Since any one of the vector operations (a)-(c) is rather simple, the CPU finishes a computation at a speed faster than that of transferring data from/to the memory, thus the CPU ends up wasting a significant fraction of time in idling. On the other hand, for the vector operation (d), the number of FPO is much more than that of any one of (a)-(c), thus when the CPU completes its operations on a portion of the vectors, the next set of data might have been ready, so the CPU does not waste much time in the memory I/O. This explains why the average CPU time per FPO of (a)-(c) is much longer than that of (d). Further, this simple picture also explains why turning on SSE2 of Pentium 4 (see Table 1) doubles the speed of (d) but has no speedups for (a)-(c), since the bottleneck of (a)-(c) is essentially due to the memory bandwidth rather than the speed of the CPU.

If the memory bandwidth is the major cause for the inefficiency of the simple vector operations (a)-(c), then using faster memories would increase the speeds of (a)-(c) more significantly than that of (d). From Table 1 we can compare the speedups of these four vector operations as the (slower) PC800 is

\(^3\)It should be emphasized that the mechanism of the interactions between the CPU and the RAM is a rather complicated process, which is beyond the scope of this paper.
Table 2: Similar to Table I except for the platforms: IBM SP2 SMP (Power 3 at 375 Mhz) with 4 Gbyte memory, and DEC alpha XP1000 (21264A at 667 Mhz) with 1.5 Gbyte memory.

| Operation | # of FPO | CPU time(ns) per FPO |
|-----------|----------|---------------------|
|           |          | IBM                | DEC                |
| (a) $|A\rangle = c_1 |A\rangle + c_2 |B\rangle$ | $72 \times N_{site}$ | 5.269 | 7.232 |
| (b) $|V\rangle = |A\rangle + c |B\rangle$ | $48 \times N_{site}$ | 10.98 | 12.91 |
| (c) $\alpha = \langle V|V\rangle$ | $36 \times N_{site}$ | 6.209 | 7.684 |
| (d) $|A\rangle = H_w |B\rangle$ | $1644 \times N_{site}$ | 2.379 | 3.054 |

replaced with (faster) PC1066. We find that the speedup for (a)-(c) is 27%, but that for (d) is only 11%. Thus the speedups are consistent with above picture.

Obviously, the inefficiency of vector operations (a)-(c) should exist in any platforms, not only for the Pentium 4 systems. To check this, we measure $t_a, t_b, t_c$ and $t_d$ for IBM SP2 SMP (Power 3 at 375 Mhz) and DEC alpha XP1000 (21264A at 667 Mhz) respectively. The results are listed in Table 2, which give

$$ n_T \simeq \begin{cases} 21, & \text{DEC alpha XP1000,} \\ 20, & \text{IBM SP2 SMP}. \end{cases} $$

(34)

Although it is impossible to go through all platforms and measure the values of $t_a, t_b$ and $t_d$ individually, it is expected that $t_a/t_d > 1$ and $t_b/t_d > 1$ (such that the inequality (30) is amply satisfied) is a common feature of most systems. In other words, we expect that the double pass is faster than the single pass for $n > n_T \simeq 12 - 25$, at least for most platforms.

Recall that in Neuberger’s test run with SGI O2000, at $n = 32$, the double pass is faster than the single pass by 30% [5]. This is not a surprise at all, in view of similar speedups of other systems at $n = 32$. For example, for IBM SP2 SMP or DEC alpha XP1000, substituting the values of $t_a, t_b, t_c$ and $t_d$ (from Table 2) into (32), we find that $S = T_1/T_2 - 1 \simeq 30\%$ at $n = 32$, which also agrees with the actual measurements given in the next section (see Table 4). Thus, the speedup $S$ of the double pass for $n > n_T$ with $n_T$ quite smaller than $n_F$ is a generic feature of any platform, stemming from the fact that the vector operations in the second pass is more efficient than those (14)-(15) in the single pass (i.e., $t_a > t_d$ and $t_b > t_d$).

Nevertheless, the salient feature of (23) and (28) is that the number of floating point operations and the CPU time for the double pass are almost independent of $n$. Thus one can choose $n$ as large as one wishes, with only a negligible overhead. For example, for the $16^3 \times 32$ lattice, with $L_i = 1000,$
$n_{ev} = 20$, and $q = 0.95$, the increment of $T_2$ from $n = 16$ to $n = 200$ is less than 0.05%. In other words, one can approximate $(H_w^2)^{-1/2}Y$ (i.e., preserve the chiral symmetry) to any precision as ones wishes, without noticeably extra costs. This is the virtue of Neuberger’s double pass algorithm, which may have been overlooked in the last five years.

4 Tests

In this section, we perform several tests on the single and the double pass algorithms, and compare the theoretical thresholds $n_T$ (29) and $n_F$ (25) with the measured values.

In Table 3, we list the number of floating point operations and the CPU time for computing one column of the inverse of

$$D(m_q) = m_q + \left(m_0 - m_q/2\right)(1 + \gamma_5S(H_w)),$$

i.e., $D^{-1}(m_q) = D(m_q)^\dagger Y$, where $Y$ is solved from

$$D(m_q)D^\dagger(m_q)Y = \left\{m_q^2 + (m_0^2 - m_q^2/4)[2 + (\gamma_5 \pm 1)S(H_w)]\right\}Y = \mathbb{I} \quad (35)$$

with multi-mass (outer) conjugate gradient for a set of 16 bare quark masses ($0.02 \leq m_q \leq 0.3$), while the inner CG (5) is iterated with the single pass and the double pass respectively. The tests are performed on the $8^3 \times 24$ lattice with SU(3) gauge configuration generated by the Wilson gauge action at $\beta = 5.8$. Other parameters are: $m_0 = 1.30$, $n_{ev} = 32$ (the number of projected eigenmodes), $\lambda_{max}/\lambda_{min} = 6.207/0.198$ (after projection), and the tolerances for the outer and inner CG loops are $1.0 \times 10^{-11}$ and $2.0 \times 10^{-12}$ respectively. The total number of iterations $L_o$ for the outer CG loop is around $100 \sim 103$, while the average number of iterations for the inner CG loop is $\sim 287$.

With the formulas (19)-(22), we can estimate the number of floating point operations and the CPU time for computing one column of $D^{-1}(m_q)$ for a number $n_q$ of bare quark masses. For the number of floating point operations, our results are

$$G_k = (L_o + n_q)F_k +$$

$$N_{site}(60L_o n_q + 84L_o + 66n_q) + 16L_o n_q - 13L_o + 18n_q + 2 \quad (36)$$

where $L_o$ is the number of iterations of the outer CG loop (35), the subscript $k = 1(2)$ stands for the single (double) pass respectively. Obviously, the most significant part of $G_k$ is the first term on the r.h.s. of (36), thus

$$G_k \simeq (L_o + n_q)F_k, \quad k = 1, 2 \quad (37)$$
Table 3: The number of floating point operations and the CPU time (in unit of second) for Pentium 4 (2.53 GHz) with one Gbyte Rambus (PC1066) to compute one column of $D^{-1}(m_q)$ for 16 quark masses, versus the degree $n$ of the rational polynomial $R^{(n-1,n)}$ in polar approximation (2).

| $n$ | Double Pass | Single Pass |
|-----|-------------|-------------|
|     | # of FPO   | CPU Time(s) | # of FPO | CPU Time(s) | $\sigma$ |
|     | $G_2$      | $V_2$ measured | $G_1$   | $V_1$ measured |    |
| 12  | $2.90 \times 10^{12}$ | 2456 | 2451 | $1.68 \times 10^{12}$ | 2342 | 2241 | $6 \times 10^{-5}$ |
| 13  | $2.90 \times 10^{12}$ | 2456 | 2452 | $1.71 \times 10^{12}$ | 2429 | 2372 | $3 \times 10^{-5}$ |
| 14  | $2.90 \times 10^{12}$ | 2456 | 2454 | $1.75 \times 10^{12}$ | 2515 | 2520 | $1 \times 10^{-5}$ |
| 16  | $2.90 \times 10^{12}$ | 2456 | 2454 | $1.81 \times 10^{12}$ | 2689 | 2714 | $3 \times 10^{-6}$ |
| 32  | $2.90 \times 10^{12}$ | 2458 | 2456 | $2.25 \times 10^{12}$ | 4097 | 4089 | $3 \times 10^{-11}$ |
| 34  | $2.90 \times 10^{12}$ | 2458 | 2458 | $2.30 \times 10^{12}$ | 4273 | 4278 | $7 \times 10^{-12}$ |
| 40  | $2.90 \times 10^{12}$ | 2458 | 2456 | $2.45 \times 10^{12}$ | 4803 | 4819 | $1 \times 10^{-13}$ |
| 56  | $2.90 \times 10^{12}$ | 2460 | 2460 | $2.86 \times 10^{12}$ | 6218 | 6261 | $2 \times 10^{-14}$ |
| 59  | $2.90 \times 10^{12}$ | 2460 | 2460 | $2.93 \times 10^{12}$ | 6483 | 6491 | $2 \times 10^{-14}$ |
| 60  | $2.90 \times 10^{12}$ | 2460 | 2461 | $2.96 \times 10^{12}$ | 6572 | 6604 | $2 \times 10^{-14}$ |
| 64  | $2.90 \times 10^{12}$ | 2460 | 2461 | $3.06 \times 10^{12}$ | 6926 | 6965 | $2 \times 10^{-14}$ |

Similarly, the most significant part of the CPU time is

$$V_k \simeq (L_o + n_q) T_k, \quad k = 1, 2.$$  (38)

where $T_1$ and $T_2$ are given in (21)-(22).

In Table 3, the estimated CPU times $V_1$ and $V_2$ are in good agreement with the measured CPU times (the deviation is always less than 5%). By comparing the CPU times for the single pass and the double pass, we see that the double pass becomes faster than the single pass at $n \simeq 13$, in agreement with the theoretical estimate (33) for $p = 0.48$, where $p$ is obtained by measuring the effective number of the $(n - 1)$ vector pairs $\{P^{(l)}, Z^{(l)}, l = 2, \ldots, n\}$ which are updated before $Z^{(l)}$ converges.

Further, comparing $G_2$ and $G_1$, we see that $G_1 \simeq G_2$ at $n_F \simeq 59$, in agreement with the theoretical estimate (26) for $p = 0.48$.

Also, in Table 3, the remarkable feature of the double pass algorithm is demonstrated: the number of floating point operations ($G_2$) and the CPU time are almost independent of $n$. Thus $n$ can be increased to 64 or any higher value such that the chiral symmetry is preserved to any precision as one wishes. The chiral symmetry breaking or the error of the rational approximation $R^{(n-1,n)}$
Table 4: The CPU time (in unit of second) for the single and the double pass algorithms to compute one column of $D^{-1}(m_q)$ for 16 quark masses, versus the degree $n$ of the rational polynomial $R^{(n-1,n)}$ in polar approximation [2].

| $n$ | P4 PC800 | IBM SP2 SMP | DEC alpha XP1000 |
|-----|----------|-------------|-------------------|
|     | 2-pass   | 1-pass      | 2-pass            | 1-pass            | 2-pass     | 1-pass |
| 20  | 4922     | 4627        | 7701              | 7674              | 9921       | 9868   |
| 21  | 4930     | 4794        | 7711              | 7881              | 9924       | 10197  |
| 22  | 4918     | 4940        | 7710              | 8090              | 9931       | 10531  |
| 24  | 4921     | 5166        | 7705              | 8529              | 9929       | 11125  |
| 26  | 4920     | 5433        | 7710              | 8990              | 9929       | 11599  |
| 32  | 4918     | 6167        | 7718              | 10138             | 9926       | 13043  |

due to a finite $n$ can be measured by

$$\sigma = \max_Y \left| \frac{W^\dagger W}{Y^\dagger Y} - 1 \right|, \quad W = S(H_w)Y,$$

(39)

which is shown in the last column of Table 3.

To check the theoretical estimates for the threshold $n_T$ in (34), we repeat the tests of Table 3 for Pentium 4 (PC800), IBM SP2 SMP, and DEC alpha XP1000 respectively. The results are listed in Table 4. Obviously, in each case, the double pass is faster than the single pass for $n > 20 \sim 22$, in good agreement with the theoretical estimates in (34). Further, at $n = 32$, the speed of the double pass is faster than the single pass by 25%, 31%, and 31% for these three platforms respectively, compatible with what Neuberger found in his test run with SGI O2000 [5]. Note that for Pentium 4, using SSE2 code increases the speedup of the double pass to 66% at $n = 32$ (see Table 3), thus makes the double pass algorithm even more favorable for P4 clusters.

At this point, it may be interesting to repeat the tests of Table 3 but replacing the polar approximation [2] with the Zolotarev optimal rational approximation,

$$S_{opt}(H_w) = h_w \sum_{l=1}^{n} \frac{b'_l}{h^2_w + c'^2_{2l-1}} \equiv H_w R^Z_{(n-1,n)}(H^2_w), \quad h_w = H_w/\lambda_{\min},$$

(40)

where

$$R^Z_{(n-1,n)}(H^2_w) = \frac{d'_0}{\lambda_{\min}} \prod_{l=1}^{n} (1 + h^2_w/c'^2_{2l-1}) = \frac{1}{\lambda_{\min}} \sum_{l=1}^{n} \frac{b'_l}{h^2_w + c'^2_{2l-1}},$$

(41)

and the coefficients $d'_0$, $b'_l$ and $c'_l$ are expressed in terms of Jacobian elliptic functions [6, 7, 8] with arguments depending only on $n$ and $\lambda^2_{\max}/\lambda^2_{\min} (\lambda_{\max}$
Table 5: The number of floating point operations and the CPU time (in unit of second) for Pentium 4 (2.53 GHz) with one Gbyte Rambus (PC1066) to compute one column of $D^{-1}(m_q)$ for 16 quark masses, versus the degree $n$ of the Zolotarev rational polynomial $R^{(n-1,n)}_Z$.

| $n$  | Double Pass |     | Single Pass |     |     |     |     | Zolotarev |
|------|-------------|-----|-------------|-----|-----|-----|-----|-----------|
|      | $\#$ of FPO | $\sigma$ | $\#$ of FPO | $\sigma$ |     |     |     |           |
|      | $G_2$       | CPU Time(s) | $G_1$       | CPU Time(s) | measured | measured |          |
| 12   | $2.90 \times 10^{12}$ | 2456 | 1.72 $\times 10^{12}$ | 2309 | 2274 | $7 \times 10^{-11}$ |
| 13   | $2.90 \times 10^{12}$ | 2456 | 1.75 $\times 10^{12}$ | 2398 | 2404 | $8 \times 10^{-12}$ |
| 14   | $2.90 \times 10^{12}$ | 2456 | 1.78 $\times 10^{12}$ | 2485 | 2463 | $1 \times 10^{-12}$ |
| 16   | $2.90 \times 10^{12}$ | 2456 | 1.83 $\times 10^{12}$ | 2659 | 2638 | $3 \times 10^{-14}$ |
| 32   | $2.90 \times 10^{12}$ | 2458 | 2.25 $\times 10^{12}$ | 4058 | 4068 | $3 \times 10^{-14}$ |
| 34   | $2.90 \times 10^{12}$ | 2458 | 2.30 $\times 10^{12}$ | 4233 | 4245 | $3 \times 10^{-14}$ |
| 40   | $2.90 \times 10^{12}$ | 2460 | 2.45 $\times 10^{12}$ | 4759 | 4795 | $3 \times 10^{-14}$ |
| 56   | $2.90 \times 10^{12}$ | 2460 | 2.86 $\times 10^{12}$ | 6159 | 6180 | $3 \times 10^{-14}$ |
| 59   | $2.90 \times 10^{12}$ | 2460 | 2.92 $\times 10^{12}$ | 6423 | 6459 | $3 \times 10^{-14}$ |
| 60   | $2.90 \times 10^{12}$ | 2460 | 2.95 $\times 10^{12}$ | 6510 | 6544 | $3 \times 10^{-14}$ |
| 64   | $2.90 \times 10^{12}$ | 2460 | 3.05 $\times 10^{12}$ | 6860 | 6903 | $3 \times 10^{-14}$ |

and $\lambda_{\text{min}}$ are the maximum and the minimum of the the eigenvalues of $|H_w|$). The results are listed in Table 5.

Comparing Table 3 with Table 5 it is clear that for the single pass with $n < 32$, Zolotarev optimal approximation is better than the polar approximation, in terms of the precision of the approximation ($\sigma$). However, for the double pass, the polar approximation seems to be as good as the Zolotarev approximation since the degree $n$ can be pushed to a very large value, with negligible extra CPU time. In other words, with the double pass algorithm, it does not matter which rational approximation one uses to compute $D^{-1}(m_q)$ in a gauge background. This seems to be a rather unexpected result.

5 Concluding remarks

So far, we have restricted our discussions to the sign function with argument $H_w$. However, it is clear that the salient features of the double pass algorithm are invariant for other choices of the argument, e.g., improved Wilson operator. In general, the double pass algorithm is a powerful scheme for the matrix-vector product $R(H^2) \cdot Y$, where $R$ can be any rational polynomial $R$ with argument $H^2$ (positive definite Hermitian operator), not just for $(H^2)^{-1/2}$. 


The virtue of Neuberger’s double pass algorithm is its constancy in speed and memory storage for any degree $n$ of the rational approximation, where its constancy in speed is valid under a mild condition ($N_{\text{site}} \gg L_i$) which can be fulfilled in most cases. Further, the double pass is faster than the single pass even for $n$ as small as 12 (Pentium 4), and it is expected that the threshold $n_T \simeq 12 - 25$ for most systems. Thus, it seems that there is not much room left for the single pass algorithm with Zolotarev approximation, unless the number of inner CG iterations is exceptionally large, which could happen if the low-lying eigenmodes of $H_w^2$ are not projected out and treated exactly.

Note that $H_w^2$ can be tridiagonalized by the conjugate gradient (6)-(11), with the unitary transformation matrix $U$ formed by the normalized residue vectors $\{\hat{R}_j, j = 0, \cdots, i\}$, and the elements of the tridiagonal matrix expressed in terms of the coefficients $\{\alpha_j, \beta_j, j = 0, \cdots, i\}$ (up to the tolerance of the conjugate gradient), i.e.,

$$U^\dagger H_w^2 U \simeq \mathcal{T}$$

(42)

where

$$U_{kj} = \frac{(R_j)_k}{\sqrt{(R_j|R_j)}} ,$$

(43)

and $\mathcal{T}$ is a symmetric tridiagonal matrix with nonzero elements

$$\mathcal{T}_{jj} = \frac{\beta_j}{\alpha_{j-1}} + \frac{1}{\alpha_j} ,$$

(44)

$$\mathcal{T}_{j+1,j} = \mathcal{T}_{j,j+1} = -\sqrt{\frac{\beta_{j+1}}{\alpha_j}}, \quad j = 0, \cdots, i.$$  

(45)

Thus, after running the first pass of the CG loop (6)-(11), $\mathcal{T}$ can be constructed from the coefficients $\{\alpha_j, \beta_j\}$, and diagonalized by an orthogonal transformation

$$\mathcal{T} = O\Lambda\hat{O} .$$

(46)

Then the matrix-vector product $(H_w^2)^{-1/2}Y$ can be evaluated as

$$\frac{1}{\sqrt{H_w^2}} Y \simeq UO \frac{1}{\sqrt{\Lambda}} \hat{O} U^\dagger Y = \sum_{j=0}^{i} l_j R_j$$

(47)

where

$$l_j = \sum_{m=0}^{i} O_{jm} \frac{1}{\sqrt{\lambda_m}} O_{0m} \sqrt{\frac{\langle R_0|R_0 \rangle}{\langle R_j|R_j \rangle}} .$$

(48)
Here the summation on the r.h.s. of (47) is obtained by running the second pass of the CG loop \{6, 7, 9, 11\}, and adding $l_j R_j$ to the sum successively from $j = 0$ to $i$.

It is well known that (any positive definite Hermitian matrix) $H^2_w$ can be tridiagonalized by Lanczos iteration \[9, 10\] as well as the conjugate gradient. The connection between the Lanczos iteration and the conjugate gradient for the tridiagonalization of a positive definite Hermitian matrix has been well established \[9\], and both have almost the same performance in practice. In Ref. \[11\], the Lanczos approach was proposed for the matrix-vector product $(H^2_w)^{-1/2} Y$, and its variant (replacing Lanczos iteration with the conjugate gradient) was used in Ref. \[12\].

The only difference between the Lanczos (CG) algorithm and Neuberger’s double pass algorithm is the diagonalization of the tridiagonal matrix $T$ and the computation of the coefficients \{6\} \[13\] in the former versus the computation of the coefficients \{7\} \[14\] in the latter. Since the number of floating point operations for the diagonalization of a symmetric tridiagonal matrix $T$ is $\approx 3L^3_i$ (where $L_i$ is the number of iterations of the inner CG loop, or the size of $T$), it is compatible with that of computing the coefficients \{7\}, i.e., the last term on the r.h.s. of (20). Thus we expect that the performance (speed and accuracy) of Lanczos (CG) algorithm and Neuberger’s double pass algorithm are compatible.

In Table 6 we compare the Lanczos (CG) algorithm with Neuberger’s double pass algorithm, by computing one column of $D^{-1}(m_q)$ (for 16 bare quark masses) on the $16^3 \times 32$ lattice with SU(3) gauge configuration generated by the Wilson gauge action at $\beta = 6.0$. Other parameters are: $m_0 = 1.30$, $n_{ev} = 20$ (the number of projected eigenmodes), $\lambda_{max}/\lambda_{min} = 6.260/0.215$ (after projection), and the tolerances for the outer and inner CG (Lanczos) loops are $1.0 \times 10^{-11}$ and $2.0 \times 10^{-12}$ respectively. The number of iterations for the outer CG loop is $L_o = 347$, while the average number of iterations for the inner CG loop is $\sim 300$. Evidently, these seemingly different algorithms have almost the same speed as well as the accuracy ($\sigma$).

Thus, for quenched lattice QCD, one has several compatible options to compute the quenched quark propagator

$$(D_c + m_q)^{-1} = (1 - rm_q)^{-1}[D^{-1}(m_q) - r] , \quad r = \frac{1}{2m_0} ,$$

even though we have chosen Neuberger’s double pass algorithm to solve $D^{-1}(m_q)$ in our recent investigation \[13\]. Nevertheless, for lattice QCD with dynamical quarks, the quark determinant $\det D(m_q)$ could not be computed directly with existing algorithms and computers. If $\det D(m_q)$ is incorporated through the dynamics of $2n$ pseudofermion fields (where $n$ can be regarded as the degree $n$ in the rational polynomial $R^{(n-1,n)}$), then an additional degree of freedom (or the fifth dimension with $N_s = 2n$ sites) has to be introduced. Thus a rele-
Table 6: The number of floating point operations and the CPU time (in unit of second) for Pentium 4 (2.53 GHz) with one Gbyte Rambus (PC1066) to compute one column of $D^{-1}(m_q)$, versus different algorithms.

|                  | Double pass algorithm | Lanczos (CG) algorithm |
|------------------|-----------------------|------------------------|
|                  | Polar($n = 128$)      | Zolotarev($n = 16$)    | Lanczos | CG          |
| FPO              | $9.49 \times 10^{13}$ | $9.49 \times 10^{13}$ | $9.54 \times 10^{13}$ | $9.51 \times 10^{13}$ |
| Time (total)     | 94543                 | 94632                  | 97824   | 94722       |
| Time (2nd pass)  | 46281                 | 46303                  | 46353   | 46174       |
| $\sigma$        | $1 \times 10^{-14}$   | $1 \times 10^{-14}$    | $1 \times 10^{-14}$ | $1 \times 10^{-14}$ |

The relevant question is how to reproduce $\det D(m_q)$ accurately with the minimal $N_s$. A solution has been presented in Ref. [14]. On the other hand, it would be interesting to see whether there is an algorithm to drive the dynamics of these $N_s$ pseudofermion fields such that the cost is almost independent of $N_s = 2n$.

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