# Construction of staples in lattice gauge theory on a parallel computer 

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#### Abstract

We propose a simple method to construct staples in lattice gauge theory with Wilson action on a parallel computer. This method can be applicable to any dimensional system and to any dimensional division without difficulty. Furthermore this requires rather small working area to realize gauge simulation on a parallel computer.


## 1. Introduction

Recently numerical simulations in lattice gauge theory become very important to investigate nonperturbative physics as well as to evaluate interesting quantities from first principle. In fact numerical studies grows with the growth of powerful computers like supercomputers and parallel computers. There are many commercial parallel computers available now as well as many dedicated QCD parallel computers. In particular many lattice QCD(Quantum Chromo Dynamics) works have been performed on parallel computers [1].

However for programmers, the variety of parallel computers prevents the portability of their code. Moreover the parallel code usually needs more working area coming from the overlapping with next processors than the code which runs on a single processor. These "portability of code" and "reducing of working area" become crucial to simulate a larger system and on a different platform.

In this paper a simple method to overcome these problems in lattice QCD Monte Carlo Simulations is proposed. The organization of this paper is as follows. In section 2, the notations and preparations which is necessary to latter presentations is introduced. Actual construction of staples on a parallel computer is presented in section 3. The summary is given in section 4.

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## 2. Notations and Preparations

Consider $d$-dimensional pure gauge theory defined on a lattice with Wilson action. Let $U_{n, \mu}$ be a link variable of gauge field connecting between site $n$ and $n+\hat{\mu}$, the staple $X_{n, \mu}$ concerning the link $U_{n, \mu}$ is

$$
\begin{align*}
X_{n, \mu} & =\sum_{\nu \neq \mu}\left(X_{n, \mu \nu}^{(+)}+X_{n, \mu \nu}^{(-)}\right)  \tag{1}\\
X_{n, \mu \nu}^{(+)} & =U_{n, \nu} U_{n+\hat{\nu}, \mu} U_{n+\hat{\mu}, \nu}^{\dagger}  \tag{2}\\
X_{n, \mu \nu}^{(-)} & =U_{n-\hat{\nu}, \nu}^{\dagger} U_{n-\hat{\nu}, \mu} U_{n-\hat{\nu}+\hat{\mu}, \nu} \tag{3}
\end{align*}
$$

making the Wilson action $S$ as
$S \propto \sum_{n, \mu} \operatorname{Re} \operatorname{Tr}\left(U_{n, \mu} X_{n, \mu}^{\dagger}\right)$.
Let $N_{\mu}(1 \leq \mu \leq d)$ be a lattice size of $\mu$ direction, then each site $x$ can be specified with its coordinate $x=\left(x_{1}, x_{2}, \ldots, x_{d}\right)\left(0 \leq x_{\mu} \leq N_{\mu}-1\right)$, and total volume is $\prod_{\mu=1}^{d} N_{\mu}$. Using these coordinates we can define a global address of site. One simple way to do this is to specify global address $j$ of site $x$ as
$j(x)=1+x_{1}+\sum_{\mu=2}^{d} x_{\mu} \prod_{k=1}^{\mu-1} N_{k}$.
Then we introduce "normal order" of sites such that sites are ordered with an increasing order of their global addresses.

In order to realize even-odd (checkerboard) decomposition of sites which is necessary for parallelization we restrict on the case that each $N_{\mu}$ is
even. We then call a site $x$ is even (odd) site if $\sum_{\mu=1}^{d} x_{\mu}$ is even (odd).

Next we put this lattice on a parallel computer which consists of $\prod_{\mu=1}^{d} M_{\mu}\left(1 \leq M_{\mu} \leq\right.$ $N_{\mu}$ ) processors, namely we consider the case that each processor is responsible for $\prod_{\mu=1}^{d} m_{\mu}\left(m_{\mu} \equiv\right.$ $\left.N_{\mu} / M_{\mu}\right)$ sites. If $M_{\mu} \neq 1, \mu$ direction diveded into $M_{\mu}$ pieces and put on multi processors. On the other hand if $M_{\mu}=1, \mu$ direction is not divided into processors but put on a single processor. In order to realize even-odd decomposition of sites also in each processor, $\prod_{i=1}^{d} m_{i}$ is restricted to be even.

From now on we restrict ourselves on a processor which is denoted by $\mathcal{P}$, but the story discussed below is universal and applicable to all processors we think. For convenience we denote a neighboring processor in $\pm \mu$ direction as $\mathcal{P} \pm \hat{\mu}$.

Then we classify all sites in $\mathcal{P}$ into two groups; one is even site group $G_{e}$ which consists of all even sites and the other is odd site group $G_{o}$ which consists of all odd sites. Since both groups have $V\left(\equiv \prod_{i=1}^{d} m_{i} / 2\right)$ elements, we can number all elements of $G_{e}\left(G_{o}\right)$ in $\mathcal{P}$ from 1 to $V$ in normal order introduced above. In terms of this numbering we can define a local address of sites in $\mathcal{P}$.

Suppose a site n is $\operatorname{in} G_{e}\left(G_{o}\right)$ and has a local address $l$. We refer the link variable $U_{n, \mu}$ as:
$U_{n, \mu}=\left\{\begin{array}{ll}E_{l, \mu} & \left(n \in G_{e}\right) \\ O_{l, \mu} & \left(n \in G_{o}\right)\end{array}\right.$,
where $E_{l, \mu}\left(O_{l, \mu}\right)$ represents a link variable attaching a even (odd) site whose address is $l$ and having a direction $\mu$.

Next we introduce a list vector $v_{e}(l, \mu)\left(v_{o}(l, \mu)\right)$ which points to a odd (even) site address located on $n+\hat{\mu}$ as a function of a even (odd) site address $l$. If $M_{\mu}=1$, a site $n+\hat{\mu}$ is also in $\mathcal{P}$. In this case $v_{e}(l, \mu)\left(v_{o}(l, \mu)\right)$ can be defined properly. If $M_{\mu} \neq 1$, however, there is a subgroup $B_{e, \mu}^{(+)}\left(B_{o, \mu}^{(+)}\right)$of $G_{e}\left(G_{o}\right)$ whose neighboring sites in $+\mu$ direction are not in $\mathcal{P}$ but in $\mathcal{P}+\hat{\mu}$, i.e.
$n \in B_{e, \mu}^{(+)} \cap G_{e} \Rightarrow n+\hat{\mu} \notin G_{o}$
$n \in \bar{B}_{e, \mu}^{(+)} \cap G_{e} \Rightarrow n+\hat{\mu} \in G_{o}$
$n \in B_{o, \mu}^{(+)} \cap G_{o} \Rightarrow n+\hat{\mu} \notin G_{e}$
$n \in \bar{B}_{o, \mu}^{(+)} \cap G_{o} \Rightarrow n+\hat{\mu} \in G_{e}$.
In this case $v_{e}(l, \mu)\left(v_{o}(l, \mu)\right)$ can not be defined properly in $\mathcal{P}$ and we must extend the definition. We introduce a new group $N_{e, \mu}\left(N_{o, \mu}\right)$ which consists of sites pointed by $n+\hat{\mu}$ where $n \in B_{e, \mu}^{(+)}$ $\left(n \in B_{o, \mu}^{(+)}\right)$. It is noted that elements of $N_{e, \mu}$ $\left(N_{o, \mu}\right)$ are not in $\mathcal{P}$, but in $\mathcal{P}+\hat{\mu}$. Here we extend the site numbering in $\mathcal{P}$ to $N_{e, \mu}\left(N_{o, \mu}\right)$, namely we number elements of $N_{e, \mu}\left(N_{o, \mu}\right)$ from $V+1$ to $V+V / m_{\mu}$ in normal order, then we can define $v_{e}(l, \mu)\left(v_{o}(l, \mu)\right)$ which points to a odd (even) site address located on $n+\hat{\mu}$ in $N_{o, \mu}\left(N_{e, \mu}\right)$.

Just like as $B_{e, \mu}^{(+)}\left(B_{o, \mu}^{(+)}\right)$, we can introduce a subgroup $B_{e, \mu}^{(-)}\left(B_{o, \mu}^{(-)}\right)$of $G_{e}\left(G_{o}\right)$ whose neighboring sites in negative $\mu$ direction are not in $\mathcal{P}$ but in $\mathcal{P}-\hat{\mu}$. Since there are $V / m_{\mu}$ sites in $B_{e, \mu}^{(-)}$ $\left(B_{o, \mu}^{(-)}\right)$, we can number these sites in $B_{e, \mu}^{(-)}\left(B_{o, \mu}^{(-)}\right)$ from $i=1$ to $V / m_{\mu}$ in normal order. If a site n in $B_{e, \mu}^{(-)}\left(B_{o, \mu}^{(-)}\right)$has a local address $l$ and specified by a number $i$ discussed above, we can introduce a new function $b_{o}(i, \mu)\left(b_{e}(i, \mu)\right)$ defined as:

$$
\begin{array}{lll}
l=b_{e}(i, \mu) & \text { in } B_{e, \mu}^{(-)}, & 1 \leq i \leq V / m_{\mu}  \tag{8}\\
l=b_{o}(i, \mu) & \text { in } B_{o, \mu}^{(-)}, & 1 \leq i \leq V / m_{\mu}
\end{array}
$$

## 3. Construction of Staples

In this section, we construct staples. For simplicity, we restrict on the case that $n \in G_{e}$.

## 3.1. positive $\nu: X_{n, \mu \nu}^{(+)}$

First we construct $X_{n, \mu \nu}^{(+)}$in two steps. We introduce temporary matrix T as:
$T=U_{n, \nu} U_{n+\hat{\nu}, \mu}$
then we construct $X_{n, \mu \nu}^{(+)}$as:
$X_{n, \mu}^{(+)}=T U_{n+\hat{\mu}, \nu}^{\dagger}$.
If $M_{\nu} \neq 1$ and in case of $n \in B_{e, \nu}^{(+)}$we do not have $U_{n+\hat{\nu}, \mu}$ in $\mathcal{P}$. Since the way to obtain information from other processors is machine dependent, in this paper we use send/receive syntax to perform inter-processor communications. We have to get $U_{n+\hat{\nu}, \mu}$ from $\mathcal{P}+\hat{\nu}$, in other words we have to send $U_{n+\hat{\nu}, \mu}$ to $\mathcal{P}-\hat{\nu}$. So we first prepare
the links that should be sent so that the links are orderd sequentially in a dimension. Second we send links prepared to $\mathcal{P}-\hat{\nu}$. Third we receive links from $\mathcal{P}+\hat{\nu}$ and store them to appropriate point of dimension.

$$
\begin{array}{lccc}
\text { PREPARE } & O_{\mu}(V+i) & \leftarrow & O_{\mu}\left(b_{o}(i, \nu)\right) \\
\text { SEND } & \text { TO } & \mathcal{P}-\hat{\nu} & O_{\mu}(V+i) \\
\text { RECEIVE } & \text { FROM } & \mathcal{P}+\hat{\nu} & O_{\mu}(V+i)
\end{array}
$$

For latter convenience, we introduce a function SETLINK that performs above three operations. The syntax is:
$\operatorname{SETLINK}\left(O_{\mu}, b_{o}, V, m_{\nu}, \nu\right)$.
Now $T$ can be made by;
$T(l)=E_{\nu}(l) O_{\mu}\left(v_{e}(l, \nu)\right), \quad 1 \leq l \leq V$.
Obviously SETLINK is not necessary if $M_{\nu}=1$.
Next we prepare $U$ s in eq.(10). If $M_{\mu} \neq 1$ first we perform SETLINK:

$$
\begin{equation*}
\operatorname{SETLINK}\left(O_{\nu}, b_{o}, V, m_{\mu}, \mu\right) \tag{13}
\end{equation*}
$$

Then we can construct $X^{(+)}$as,
$X_{l, \mu \nu}^{(+)}=T(l) O_{\nu}^{\dagger}\left(v_{e}(l, \mu)\right), \quad 1 \leq l \leq V$.
3.2. negative $\nu: X_{n, \mu \nu}^{(-)}$

To calculate $X_{n, \mu \nu}^{(-)}$we use a technique. First construct $X_{n, \mu \nu}^{(-)}$as $n-\hat{\nu}$ are the starting points. Next we move staples to $+\nu$ direction and obtain $X_{n, \mu \nu}^{(-)}$. Just like as $X_{n, \mu \nu}^{(+)}$case, we do in two steps. Since $n-\hat{\nu}$ are odd sites, temporal matrix T which is the products of first two matrix of the right hand site of eq.(3) can be construct as;

$$
\begin{align*}
& T(l)=O_{\nu}^{\dagger}(l) O_{\mu}(l), \quad 1 \leq l \leq V  \tag{15}\\
& \quad \text { If } M_{\mu} \neq 1 \text { do }
\end{align*}
$$

$$
\begin{equation*}
\operatorname{SETLINK}\left(E_{\nu}, b_{e}, V, m_{\mu}, \mu\right) \tag{16}
\end{equation*}
$$

We then get $W(l)$ as;

$$
\begin{equation*}
W(l)=T(l) E_{\nu}\left(v_{o}(l, \mu)\right), \quad 1 \leq l \leq V \tag{17}
\end{equation*}
$$

which corresponds $X_{n, \mu \nu}^{(-)}$but $n-\hat{\nu}$ are the starting points instead of $n \mathrm{~s}$. Next we move $W(l)$ to $+\nu$ direction;
$T\left(v_{o}(l, \nu)\right) \leftarrow W(l), \quad 1 \leq l \leq V$.

If $M_{\nu} \neq 1$ above $+\nu$ operation require interprocessor communications. This can be done by sending $T(n+\nu)\left(n \in N_{e, \nu}\right)$ to $\mathcal{P}+\hat{\nu}$ and by receiving them from to $\mathcal{P}-\hat{\nu}$ and storing them to $T(n)\left(n \in B_{e, \nu}^{(-)}\right)$.

| SEND | TO | $\mathcal{P}+\hat{\nu}$ | $T(V+i)$ |
| :--- | :---: | :---: | :---: |
| RECEIVE | FROM | $\mathcal{P}-\hat{\nu}$ | $T(V+i)$ |
| STORE | $T\left(b_{e}(i, \nu)\right)$ | $\leftarrow$ | $T(V+i)$ |

This gives $X_{l, \mu \nu}^{(-)}$;
$X_{l, \mu \nu}^{(-)}=T(l), \quad 1 \leq l \leq V$.
Just like as SETLINK, it is useful to introduce a function SLIDEMATRIX that performs above three operations. The syntax is:
$\operatorname{SLIDEMATRIX}\left(T, b_{e}, V, m_{\nu}, \nu\right)$.

## 4. Summary

We have applied this method both on Fujitsu AP1000 at Fujitsu Parallel Computing Research Facilities and on Intel Paragon at Institute for Numerical Simulations and Applied Mathematics in Hiroshima University. We have checked that this method can be applicable to any dimensional system and to any dimensional division of the original system without any difficulty. Reduction of working area has been performed nicely compared with a original program which uses overlapping with next processors. We hope that this method will be a good help for beginners of parallel programming.

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