A new lattice gauge action without scaling artifacts

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(October 3, 2004)

Abstract

I describe a new way of constructing a gauge action that eliminates scaling artifacts, by writing the continuum formalism in terms of “gauge links” (Schwinger line integrals) and using the optimal SLAC representation of the lattice derivative. Computational performance can be maintained by implementing the action as a “stochastic” operator, as has been recently implemented in the MILC code for the optimal D-slash operator and the antialiasing filter.

1. Introduction

I recently proposed a new paradigm for lattice calculations that addresses a number of fundamental flaws in current practice. Until now, fields have been multiplied together in position space without any pre-filtering or post-filtering. But it is a fundamental result of Fourier theory that such unfiltered products will automatically “foul themselves”, because high-momentum modes in the product “fold back” from the Brillouin zone boundary and “masquerade” or “alias” as low-momentum modes (see, e.g., [1]). This “fouling” occurs every time that a product of fields is formed—which in the context of lattice field theory means at practically every step. That practitioners have managed to extract meaningful numbers from the resulting mess is close to miraculous—and it has only been achieved by using enormously large lattices and intricate extrapolation procedures.

Some have discovered, empirically, that high momentum modes constitute more noise than signal, because the more they “fatten” or “smear” the links and operators, the better the signal-to-noise ratio has become. But the correct solution, that eliminates the mess before it happens, is to apply an “antialiasing filter” to each field, at each and every stage, that has no effect on any momentum mode with $|p_\mu| < 2\pi/3a$, but eliminates all modes outside this window [2]. Such a filter has now been implemented, for both scalar and parallel computation, using the public-domain MILC code [3], with performance being maintained by implementing the operator in a “stochastic” fashion [4], where we can “dial” the stochasticity from zero (fully deterministic) to as high as we like (every coefficient interpreted as a probability).

Likewise, until now the representation of fermions on the lattice has been woefully inadequate. The use of “ultralocal” derivative operators was originally mandated by performance considerations, and by the Nielsen–Ninomiya theorem locked practitioners into a no-win situation of having to deal with either doubled fermions or destroyed chiral properties. The
development of Ginsparg–Wilson fermions has begun to break down the myth of the need for ultralocality. However, I have argued [4, 6] that the correct way to proceed is to simply use the “SLAC” derivative operator [5], which is defined to have a perfect representation in momentum space (within the first Brillouin zone). The SLAC operator seems to have been tried and discarded long ago, and there is resistance to it being resurrected. However, the reason for it being discredited is now easy to discern. By definition, the momentum modes of the SLAC derivative operator with largest magnitude are those near the Brillouin zone boundary (simply because it is defined to be $ip_\mu$ in momentum space). Without any antialiasing filters, these dominant modes will be aliased right down to low momentum values, with just a single $D$-slash operation. Extracting any meaningful signal from beneath this aliasing noise becomes impossible. Ironically, the very weakness of an ultralocal derivative operator that causes the doubling problem in the first place—the fact that it must vanish somewhere other than $p = 0$, usually at the Brillouin zone boundary—coincidentally provides an (incomplete) filtering of high-momentum modes, which makes its performance appear superior to the SLAC operator, if no antialiasing filters are applied.

Removing this illusory disadvantage with a properly antialiased lattice engine, we still have to face the question of performance and cost. The SLAC derivative operator connects every site to every other site along the direction of the derivative. Here, again, the implementation of the operator in a “stochastic” fashion solves the problem, allowing the operator to perform perfectly in the mean, where we can dial the amount of “stochasticity” by trading performance off against noise, ultimately finding the setting that optimizes our computing power. This optimal $D$-slash operator has also been recently implemented for both scalar and parallel computations, using the MILC code [3].

The construction of these two important planks in the new lattice paradigm begs a tantalizing question: Is it possible to construct a lattice engine that has no inherent scaling artifacts at all? Such a computation engine would be the Holy Grail of lattice research. The only effects of the finiteness of the lattice would be physical ones: the “squeezing” of states (if the lattice is too small, in its overall dimensions), and the elimination (regulation) of high-momentum modes, for any finite value of $a$. The former is expected to fall off exponentially, provided that the overall dimensions of the lattice are sufficiently large (a few fm or more in each direction); the latter represents the effects of regulation and renormalization, that are fundamental to the physical description.

Can such an engine be constructed? With an optimal $D$-slash operator, and an antialiasing filter, the only part of a lattice computation retaining scaling artifacts is the evaluation of the gauge action. Now, the lowest-approximation plaquette estimate has been “improved” in numerous ways over the years, but, again, the gospel of ultralocality has dominated. Generally, a few higher-order strings of links have been introduced, with their coefficients manually matched up to provide a cancellation of artifacts to some order in $a$. Some of these improvements also mix in the dynamics, to provide better cancellation.

But is there no simple way to systematically derive all of the required strings of links? Consider: if we actually represented the gauge field by the $A_\mu$, rather than links, then all we would need to do would be to compute $F_{\mu\nu}$ by means of derivative operations (and a commutator), and we already know the optimal way to perform a derivative (the SLAC operator). Moreover, this would be a manifestly two-dimensional problem: you only compute this “curl”, namely, $F_{\mu\nu}$, two dimensions at a time. Of course, we don’t represent the gauge
field by the $A_\mu$, because we want to maintain gauge invariance identically—that’s why we use the links. But the links are derived fairly simply from the $A_\mu$; so is there a way to algorithmically construct a gauge action with a perfect dispersion relation (within the first Brillouin zone) by using derivative operations on the link description itself?

In the following sections I will argue that the answer to this question is “yes”. In Sec. 2 I show how the continuum gauge theory can be rewritten in terms of “links” (i.e., Schwinger line integrals) instead of the $A_\mu$, where derivative operations are applied to shift the endpoints of these links infinitesimally. In Sec. 3 I then show how the SLAC derivative operator can be used to optimally represent this continuum description on the lattice, with each contribution being a closed string of gauge links; in other words, gauge invariance is maintained for each and every contribution. The evaluation of these closed strings can then be performed stochastically, in the same way that the antialiasing and optimal $D$-slash operations have already been implemented in the MILC code.

2. Continuum gauge theory using links

Consider the Schwinger line integral $U(y, x, P)$ along a path $P$ between spacetime points $x$ and $y$:

$$U(y, x, P) \equiv \mathcal{P} \exp\left(ig \int_{P}^{y} dz^\mu A_\mu(z)\right), \quad (1)$$

where

$$A_\mu(x) \equiv T_b A^b_\mu(x)$$

is the gauge field, the $T_b$ are the generators of the gauge group, $g$ is the bare coupling constant of the gauge interaction, and the path-ordering operator $\mathcal{P}$ ensures that products of non-Abelian quantities arising from the exponentiation operation are correctly arranged according to the order that they are encountered along the path of integration. The links of lattice gauge theory are simply Schwinger line integrals of length $a$ along the four principal lattice directions; in other words, Schwinger line integrals are “continuum links”.

Under a gauge transformation, $U(y, x, P)$ transforms at the endpoints $x$ and $y$, oppositely to $\psi(x)$ and $\bar{\psi}(y)$ respectively, so that the quantity

$$\bar{\psi}(y) U(y, x, P) \psi(x) \quad (2)$$

is gauge-invariant, as is

$$\text{Tr} U(x, x, P), \quad (3)$$

for any closed path $P$ leading from $x$ back to $x$.

Consider, now, the “partial derivative”

$$\frac{\partial}{\partial x^\mu} U(y, x, P),$$
obtained by shifting the endpoint \( x \) by a small amount \( \delta x^\mu \) in the \( \mu \)-direction, with the \( x \)-end of the path \( P \) being extended by this additional displacement \( \delta P^\mu \equiv \hat{\delta}x^\mu \), and using first principles to compute the “derivative”:

\[
\frac{\partial}{\partial x^\mu} U(y, x, P) \equiv \lim_{\delta x^\mu \to 0} \frac{U(y, x + \delta x^\mu, P + \delta P^\mu) - U(y, x, P)}{\delta x^\mu}.
\]  

(4)

It is clear from (1) that

\[
\frac{\partial}{\partial x^\mu} U(y, x, P) = -igU(y, x, P) A_\mu(x),
\]  

(5)

from the fundamental definition of integration, and the path-ordering operator \( \mathcal{P} \).

Consider, now, the quantity

\[
C_F(x) \equiv i \frac{\partial}{\partial x^\mu} \bar{\psi}(y) \gamma^\mu U(y, x, P) \psi(x) \bigg|_{y \to x, P \to 0},
\]  

(6)

where the point \( y \) is brought into coincidence with the point \( x \) after the differentiation with respect to \( x^\mu \) has been performed, and where in writing \( P \to 0 \) we are implying that the length of the path \( P \) from \( x \) to \( y \) shrinks to zero as \( y \) approaches \( x \); i.e., there is no “loop” of \( P \) left outside the point \( x \) when we take the limit. Using the product rule of differentiation, and noting that \( \bar{\psi}(y) \) is independent of \( x \), we find that (6) becomes

\[
C_F(x) = i \left\{ \bar{\psi}(y) \gamma^\mu \left[ \frac{\partial}{\partial x^\mu} U(y, x, P) \right] \psi(x) + \bar{\psi}(y) \gamma^\mu U(y, x, P) \frac{\partial}{\partial x^\mu} \psi(x) \right\} y \to x, P \to 0.
\]

Substituting the result (5) for the expression in brackets, we then find that

\[
C_F(x) = \left\{ g \bar{\psi}(y) \gamma^\mu U(y, x, P) A_\mu(x) \psi(x) + i \bar{\psi}(y) \gamma^\mu U(y, x, P) \frac{\partial}{\partial x^\mu} \psi(x) \right\} y \to x, P \to 0.
\]

The quantity \( U(y, x, P) \) is now no longer being differentiated, and so we can immediately take the limit \( y \to x \) with \( P \to 0 \). Noting that

\[
U(y, x, P) \bigg|_{y \to x, P \to 0} \equiv 1,
\]

we therefore find that

\[
C_F(x) = i \bar{\psi}(x) (\hat{\delta} - igA) \psi(x) \equiv i \bar{\psi}(x) \hat{D} \psi(x),
\]  

(7)

namely, the fermion \( D \)-slash part of the Lagrangian.

Eq. (6) thus tells us how to construct the fermion part of the continuum Lagrangian out of links, rather than the \( A_\mu \): Join \( \bar{\psi}(y) \) to \( \psi(x) \) with a \( \gamma^\mu \) and a gauge link from \( y \) to \( x \) sandwiched in between, then take the “partial derivative” \( \partial/\partial x^\mu \), with the link attached, and then finally bring \( y \) into coincidence with \( x \).

Now consider

\[
C_G(x) \equiv \left( \frac{\partial}{\partial x^\mu} \frac{\partial}{\partial x^\nu} - \frac{\partial}{\partial x^\nu} \frac{\partial}{\partial x^\mu} \right) \left( \frac{\partial}{\partial y_\alpha} \frac{\partial}{\partial y_\beta} - \frac{\partial}{\partial y_\beta} \frac{\partial}{\partial y_\alpha} \right) \text{Tr} \left. U(y, x, P) \right|_{y \to x, P \to 0}.
\]  

(8)
which is gauge-invariant when the points $x$ and $y$ are brought into coincidence in the final limit, creating a closed link loop. (Note that these “partial derivatives” do not commute, because each actually represents the shifting of an endpoint and the extension of the path of the link.) Now, acting on the result (5) with the operator $\partial/\partial x^\nu$, the product rule yields in the first instance

$$\frac{\partial}{\partial x^\nu} \frac{\partial}{\partial x^\mu} U(y, x, P) = -ig \left\{ \frac{\partial}{\partial x^\nu} U(y, x, P) A_\mu(x) - ig U(y, x, P) \frac{\partial}{\partial x^\nu} A_\mu(x) \right\} .$$

We can now substitute (5) itself in for the expression in braces, to obtain

$$\frac{\partial}{\partial x^\nu} \frac{\partial}{\partial x^\mu} U(y, x, P) = -ig U(y, x, P) \left\{ \partial_\nu A_\mu(x) - i g A_\nu(x) A_\mu(x) \right\},$$

where we can use the shorthand $\partial_\nu \equiv \partial/\partial x^\nu$ inside the braces because everything in there is a function of $x$ only; the $y$-dependence of (9) is now encapsulated completely in the link $U(y, x, P)$. We thus find that

$$\left( \frac{\partial}{\partial x^\mu} \frac{\partial}{\partial x^\nu} - \frac{\partial}{\partial x^\nu} \frac{\partial}{\partial x^\mu} \right) U(y, x, P) = -ig U(y, x, P) \left\{ \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) - ig [A_\mu(x), A_\nu(x)] \right\} .$$

We now note that the expression in braces is just the definition of $F_{\mu\nu}(x)$:

$$F_{\mu\nu}(x) \equiv \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) - ig [A_\mu(x), A_\nu(x)] ,$$

so that

$$\left( \frac{\partial}{\partial x^\mu} \frac{\partial}{\partial x^\nu} - \frac{\partial}{\partial x^\nu} \frac{\partial}{\partial x^\mu} \right) U(y, x, P) = -ig U(y, x, P) F_{\mu\nu}(x) .$$

The $y$-derivatives in (8) similarly spit out a factor of $F_{\mu\nu}(y)$, so that, when we take the limit $y \to x$ with $P \to 0$, we obtain

$$C_G(x) \equiv -g^2 \text{Tr} F_{\mu\nu}(x) F^{\mu\nu}(x) .$$

In other words, the pure gauge part of the action is simply proportional to $C_G(x)$ of (8), which is constructed from an infinitesimal link, by shifting each endpoint in both the $\mu$ and $\nu$ directions, forming the appropriate commutators of these “derivatives”, and then bringing the two ends of the infinitesimal link together into a gauge-invariant loop.

### 3. Implementing the gauge action optimally on the lattice

In the previous section we found that the Lagrangian of a continuum gauge theory can be written completely in terms of the fermion fields and “continuum links” (Schwinger line integrals), without need to explicitly use the conventional gauge field $A_\mu$ at all. When we sample this formalism onto the lattice, we continue to have use of the discrete links

$$U_\mu(x) \equiv U(x + a\hat{\mu}, x, P_{x,x+a\hat{\mu}}) ,$$

which is gauge-invariant when the points $x$ and $y$ are brought into coincidence in the final limit, creating a closed link loop. (Note that these “partial derivatives” do not commute, because each actually represents the shifting of an endpoint and the extension of the path of the link.) Now, acting on the result (5) with the operator $\partial/\partial x^\nu$, the product rule yields in the first instance

$$\frac{\partial}{\partial x^\nu} \frac{\partial}{\partial x^\mu} U(y, x, P) = -ig \left\{ \frac{\partial}{\partial x^\nu} U(y, x, P) A_\mu(x) - ig U(y, x, P) \frac{\partial}{\partial x^\nu} A_\mu(x) \right\} .$$

We can now substitute (5) itself in for the expression in braces, to obtain

$$\frac{\partial}{\partial x^\nu} \frac{\partial}{\partial x^\mu} U(y, x, P) = -ig U(y, x, P) \left\{ \partial_\nu A_\mu(x) - i g A_\nu(x) A_\mu(x) \right\} ,$$

where we can use the shorthand $\partial_\nu \equiv \partial/\partial x^\nu$ inside the braces because everything in there is a function of $x$ only; the $y$-dependence of (9) is now encapsulated completely in the link $U(y, x, P)$. We thus find that

$$\left( \frac{\partial}{\partial x^\mu} \frac{\partial}{\partial x^\nu} - \frac{\partial}{\partial x^\nu} \frac{\partial}{\partial x^\mu} \right) U(y, x, P) = -ig U(y, x, P) \left\{ \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) - ig [A_\mu(x), A_\nu(x)] \right\} .$$

We now note that the expression in braces is just the definition of $F_{\mu\nu}(x)$:

$$F_{\mu\nu}(x) \equiv \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) - ig [A_\mu(x), A_\nu(x)] ,$$

so that

$$\left( \frac{\partial}{\partial x^\mu} \frac{\partial}{\partial x^\nu} - \frac{\partial}{\partial x^\nu} \frac{\partial}{\partial x^\mu} \right) U(y, x, P) = -ig U(y, x, P) F_{\mu\nu}(x) .$$

The $y$-derivatives in (8) similarly spit out a factor of $F_{\mu\nu}(y)$, so that, when we take the limit $y \to x$ with $P \to 0$, we obtain

$$C_G(x) \equiv -g^2 \text{Tr} F_{\mu\nu}(x) F^{\mu\nu}(x) .$$

In other words, the pure gauge part of the action is simply proportional to $C_G(x)$ of (8), which is constructed from an infinitesimal link, by shifting each endpoint in both the $\mu$ and $\nu$ directions, forming the appropriate commutators of these “derivatives”, and then bringing the two ends of the infinitesimal link together into a gauge-invariant loop.
where \( P_{x,x+a\hat{\mu}} \) is a straight-line path from the site at position \( x \) to the adjacent site in the \( \mu \)-direction at position \( x + a\hat{\mu} \).

For the fermionic \( D \)-slash part of the action, the expression (6) tells us to join \( \bar{\psi}(y)\gamma^\mu \) to \( \psi(x) \) with a link, and then to take the “derivative” with respect to \( x^\mu \), after which we can put \( y \) back at the position \( x \). A moment’s thought shows that this is precisely what we already do on the lattice, when we use the naive derivative or Wilson fermions: when we take the discrete derivative of \( \psi(x) \), we join it back to the \( \bar{\psi}(x)\gamma^\mu \) with the appropriate link matrices. Using the SLAC derivative simply requires that each term of \( \partial_\mu \psi \) be connected back to \( \bar{\psi}(x)\gamma^\mu \) with the appropriate link—which will, for distances greater than one lattice unit, consist of products of the elementary links (12). A stochastic implementation of this operator will not threaten gauge invariance, because each term is separately connected back to \( \bar{\psi}(x)\gamma^\mu \) with the appropriate link. This is, in fact, precisely how the operator has now been implemented in the MILC code. (To ensure maximal performance, the “integrals” of the links along each coordinate direction are first computed, so that the extraction of these “long links” reduces to simply a reading of these “integrated links” at the endpoints, sometimes supplemented by the use of a “Wilson line” if the link goes “around the back” of the lattice.)

The same thing can be done with the expression (8) for the pure gauge part of the action. If we expand out the parentheses we obtain four terms, corresponding to the derivatives at the \( x \) and \( y \) ends being taken in opposite orders, and the path-reversals of these two combinations. As with the fermionic action (6), we are free to apply whichever definition of the derivative operator we desire.

Even the naive derivative operator provides a richer variety of contributions than what one might expect. Clearly, some of the resulting diagrams will correspond to the usual plaquette contributions. Others will enclose no area whatsoever (the shifted endpoints will retrace each other), and thus simply contribute to the constant term which the sum of plaquettes is subtracted from. Over and above these lowest-order contributions, however, we also obtain rectangles covering two lattice rectangles, as well as “bow tie” and “collar” diagrams, in which we somehow have to decide how to connect the two ends that are displaced diagonally from each other.

The simplest ansatz to apply in this case—and the only one that is computationally feasible for higher-order diagrams—is that an unspecified link is split into two equal contributions, one which tracks from \( x \) to \( y \) along the \( \mu \)-direction and then the \( \nu \)-direction, and the other which tracks from \( x \) to \( y \) along the \( \nu \)-direction and then the \( \mu \)-direction. If we make this ansatz, then no diagram requires the use of more than six (long) lattice links, regardless of whether we use the naive derivative or the optimal SLAC derivative. This not only makes the calculation of each diagram computationally simple (provided that we have available the “integrated long link” library described above, as has already been implemented in the MILC code), but moreover allows the diagrams to be generated, sorted, simplified and stored efficiently.

This latter consideration is of importance to us if we wish to use the SLAC derivative, in order to eliminate scaling artifacts, because the expression (8) requires the use of four derivative operators, which implies that the number of possible diagrams is of the same order of magnitude as the total number of sites on the lattice. Clearly, a stochastic implementation of the operator is called for! Fortunately, the coefficients for the bulk of these diagrams are
as small as the diagrams themselves are numerous, precisely because the coefficient of each term in the SLAC derivative operator falls off inversely with distance. In practice, it may prove worthwhile to truncate the number of stored diagrams, so that those with a coefficient smaller than some threshold are simply discarded, because they contribute so negligibly on the average, compared to the other sources of noise in the Monte Carlo process. However, this is a practical trade-off that can be experimented with when the operator has been implemented; there is no algorithmic or computational obstacle to computing and storing all diagrams, provided that the list is sorted in decreasing order of probability (as is currently done with the stochastic $D$-slash and antialiasing operators), because in the vast majority of cases the vast bulk of this list will never be traversed.

4. Conclusions

I have argued in this paper that it is possible to construct the third and final plank of a new paradigm for lattice computations, that holds out the promise of yielding results that do not possess any scaling artifacts over and above those physically created by putting gauge theory onto a finite lattice.

This third plank will be implemented shortly using the MILC code, and put together with the optimal $D$-slash and antialiasing filters. Physics results are expected by mid-2005.

Acknowledgments

This work was in part based on the MILC collaboration’s public lattice gauge theory code. See [3]. Helpful discussions with A. A. Rawlinson, B. H. J. McKellar, C. Davies, H. Neuberger and D. Koks are gratefully acknowledged.

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