Gauge actions in openQCD simulations

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1. Introduction

The gauge actions supported in the openQCD package include the Wilson plaquette action, the tree-level Symanzik improved action and related actions. In this note, the actions are defined and the computation of the molecular-dynamics forces deriving from them is briefly discussed. The notation and the normalization conventions are the same as in refs. [1,2].

2. Definition

Let $\mathcal{S}_0$ and $\mathcal{S}_1$ be the sets of oriented plaquette and double-plaquette loops on the lattice (see fig. 1). The supported gauge actions are of the form

$$S_{\mathrm{G}} = \frac{1}{g_0^2} \sum_{k=0}^{1} c_k \sum_{\mathcal{C} \in \mathcal{S}_k} w_k(\mathcal{C}) \operatorname{tr}\{1 - U(\mathcal{C})\}, \tag{2.1}$$

where $U(\mathcal{C})$ denotes the ordered product of the link variables $U(x, \mu)$ around $\mathcal{C}$ and $w_k(\mathcal{C})$ is a weight factor specified below. In order to ensure the correct normalization of the bare coupling g_0, the coefficients c_k must be such that

$$c_0 + 8c_1 = 1. \tag{2.2}$$

Moreover, the constraint $c_0 > 0$ is imposed as otherwise there may be fields with lowest action which are not pure gauge configurations (cf. ref. [3]).
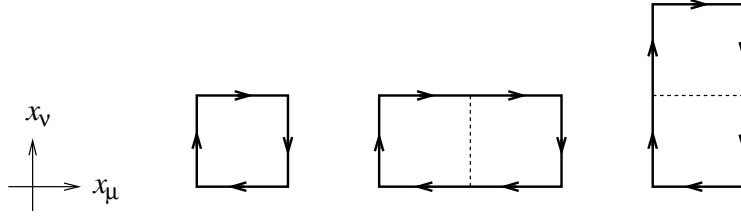
Fig. 1. Plaquette and planar double-plaquette loops in a (μ, ν)–plane of the lattice. The sums in eq. (2.1) run over all these loops, where loops differing by their orientation are considered to be different. Only those loops are included in the sums which are contained in the range $0 \leq x_0 \leq T$ of time x_0.

The weight factors $w_k(\mathcal{C})$ in eq. (2.1) are equal to 1 except for the space-like loops $\mathcal{C}$ on the boundaries of the lattice at time 0 and T, where

$$w_k(\mathcal{C}) = \tfrac{1}{2}c_{\mathrm{G}}. \tag{2.3}$$

As previously discussed in ref. [1], the coefficient c_{G} is required for O(a) improvement of correlation functions involving fields close to or at the boundaries of the lattice. In particular, setting $c_{\mathrm{G}} = 1$ ensures on-shell improvement at tree-level of perturbation theory.

In the case of the Wilson plaquette action,

$$c_0 = 1, \quad c_1 = 0, \tag{2.4}$$

while the tree-level Symanzik improved action is obtained by setting [4]

$$c_0 = \tfrac{5}{3}, \quad c_1 = -\tfrac{1}{12}. \tag{2.5}$$

Another choice of the coefficients,

$$c_0 = 3.648, \quad c_1 = -0.331, \tag{2.6}$$

was proposed by Iwasaki on the basis of a renormalization-group analysis of the pure gauge theory [5]. In the openQCD main programs, the coefficient c_0 is an adjustable parameter so that one is free to choose any one of these popular actions.
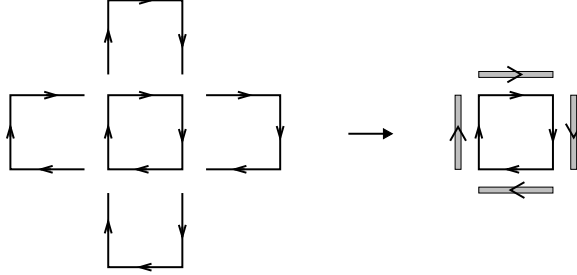
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Fig. 2. In total, there are ten oriented plaquette and planar double-plaquette loops that pass through all corners of given plaquette. The computation of the force along the edges of the plaquette deriving from these loops can be simplified by first calculating the staples shown in this figure and saving them in a temporary array (fat links on the right).

3. Computation of the gauge force

There are probably many good ways to calculate the force field

$$F^a(x, \mu) = \partial_{x,\mu}^a S_{\mathrm{G}}. \tag{3.1}$$

The method described in the following proceeds from one plaquette to the next and accumulates the contributions to the force components at the edges of the plaquette which derive from the loops that pass through all corners of the plaquette (see fig. 2).

By reversing the orientation of a given loop $\mathcal{C}$ one obtains a different loop $\mathcal{C}'$. The contribution to the gauge action of such a pair of loops is

$$s(\mathcal{C}) = \frac{2}{g_0^2} c_k w_k(\mathcal{C}) \operatorname{Re} \operatorname{tr}\{1 - U(\mathcal{C})\}, \tag{3.2}$$

where $k = 0$ or 1 depending on whether $\mathcal{C}$ is a plaquette or double-plaquette loop. Now if $\mathcal{C}$ passes through the link (x, μ) in the direction from $x + \hat{\mu}$ to x, the dependence of the action (3.2) on the link variable $U(x, \mu)$ is made explicit by

$$s(\mathcal{C}) = -\frac{2}{g_0^2} c_k w_k(\mathcal{C}) \operatorname{Re} \operatorname{tr}\{U(x, \mu) V(x, \mu; \mathcal{C})\} + \text{constant}, \tag{3.3}$$

$V(x, \mu; \mathcal{C})$ being the product of the other link variables on the loop. Similarly, if the loop passes through the link in the opposite direction, the action may be written in
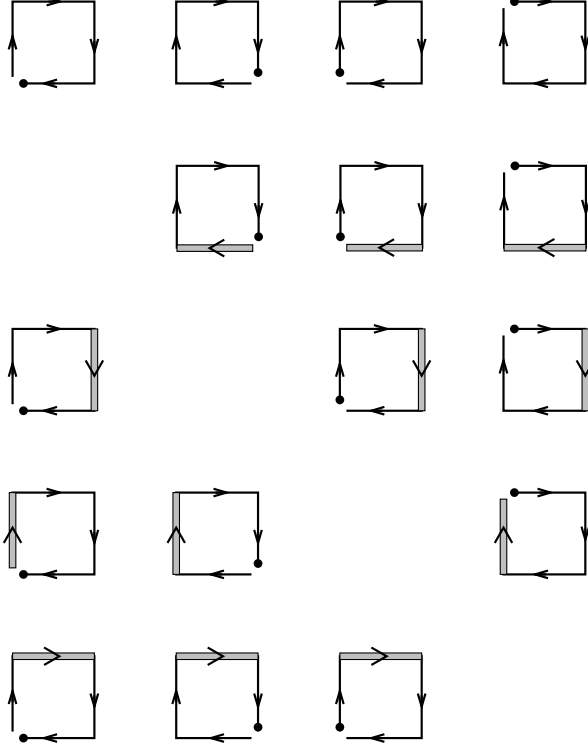
Fig. 3. Products $U(\mathcal{C})$ of link variables that contribute to the force field at the edges of the current plaquette. The dot indicates which edge is concerned and also coincides with the point x in eqs. (3.5),(3.6). The contributions from the loops on the first row must be multiplied by $\pm g_0^{-2} c_0 w_0(\mathcal{C})$ and those from all other loops by $\pm g_0^{-2} c_1 w_1(\mathcal{C})$.

the form

$$s(\mathcal{C}) = -\frac{2}{g_0^2} c_k w_k(\mathcal{C}) \operatorname{Re} \operatorname{tr}\{V(x,\mu;\mathcal{C}) U(x,\mu)^{-1}\} + \text{constant}. \tag{3.4}$$

The contribution $f(x,\mu)$ of these terms to the total force $F(x,\mu) = F(x,\mu)^a T^a$ is

$$f(x,\mu) = +\frac{1}{g_0^2} c_k w_k(\mathcal{C}) \mathcal{P}\{U(\mathcal{C})\}, \tag{3.5}$$

$$f(x,\mu) = -\frac{1}{g_0^2} c_k w_k(\mathcal{C}) \mathcal{P}\{U(\mathcal{C})\}, \tag{3.6}$$

respectively, where $U(\mathcal{C})$ is the product of the link variables around $\mathcal{C}$ starting and
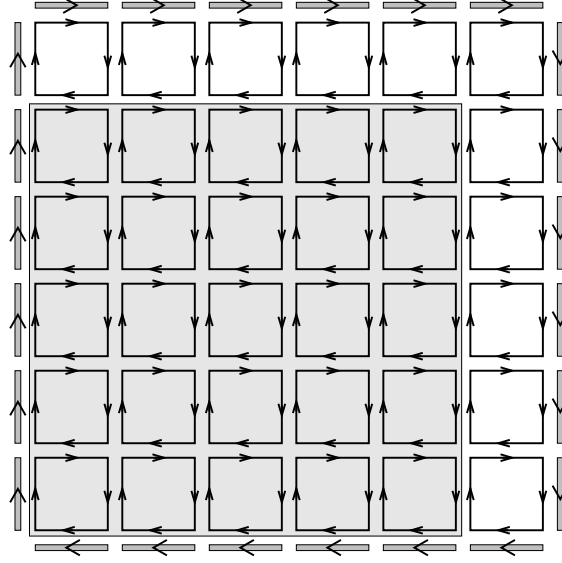
Fig. 4. Plaquettes in a two-dimensional plane of a 6^4 local lattice. The plaquettes that are fully contained in the local lattice are those in the grey square. Half of the link variables on the edges of the other plaquettes must be fetched from the neighbouring MPI processes. The staples (fat links) at the exterior boundary of the set of plaquettes shown in the figure must be copied from the neighbouring lattices too.

ending at x, while

$$\mathcal{P}\{M\} = \tfrac{1}{2}(M - M^\dagger) - \tfrac{1}{6}\mathrm{tr}(M - M^\dagger) \qquad (3.7)$$

projects any 3×3 matrix M to the Lie algebra of SU(3).

The computation of the force field may thus proceed in the following steps:

(1) Run through all unoriented plaquettes of the lattice. At a given plaquette, choose one of the two possible orientations.

(2) Consider the plaquette and double-plaquette loops that pass through all corners of the current plaquette and that have the chosen orientation. Compute the staples (fat links) shown in fig. 2.

(3) Compute the plaquette loops plotted in fig. 3 and add or subtract the associated force contribution to the force field according to eqs. (3.5),(3.6).

In step (3), the number of SU(3) multiplications can be significantly reduced by factoring common products.

4. Communication requirements

In the openQCD simulation programs, the local lattices (the parts of the full lattice on which a given MPI process operates) do not contain all the link variables required for the computations described in the previous section.

A double-counting of plaquettes can be avoided by locally running through all (x, μ, ν)–plaquettes, where x is in the local lattice and $\mu, \nu = 0, \ldots, 3$, $\mu < \nu$. The link variables on the edges of these plaquettes, which are not part of the local gauge field, must then first be copied from the neighbouring processes (see fig. 4). After that it is still not possible to compute all staples locally, but the missing ones can be calculated on the neighbouring lattices and be communicated to the local process (fat links in fig. 4). It is advantageous to store the copied staples in a buffer before the calculation of the force starts.

References

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[5] Y. Iwasaki, *Renormalization group analysis of lattice theories and improved lattice action. II – Four-dimensional non-Abelian SU(N) gauge model*, preprint UTHEP-118 (1983) [arXiv:1111.7054v1]