

cuLGT: Lattice Gauge Fixing on GPUs

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We adopt CUDA-capable Graphic Processing Units (GPUs) for Landau, Coulomb and maximally Abelian gauge fixing in 3+1 dimensional SU(3) and SU(2) lattice gauge field theories. A combination of simulated annealing and overrelaxation is used to aim for the global maximum of the gauge functional. We use a fine grained degree of parallelism to achieve the maximum performance: instead of the common 1 thread per site strategy we use 4 or 8 threads per lattice site. Here, we report on an improved version of our publicly available code (www.cuLGT.com) which again increases performance and is much easier to include in existing code. On the GeForce GTX 580 we achieve up to 470 GFlops (utilizing 80% of the theoretical peak bandwidth) for the Landau overrelaxation code.

1 Introduction

In lattice QCD, gauge fixing is necessary to study the fundamental (gauge-variant) two point functions of QCD and to compare with continuum results. Lattice gauge fixing is an optimization problem with very many degrees of freedom and many local maxima. Each local maximum corresponds to a so-called Gribov copy. These Gribov copies may have an effect on gauge-variant quantities. One way to get a unique gauge copy is to search for the global maximum of the functional. This task is very time-consuming and an efficient implementation on modern hardware is desirable. Since the optimization algorithms are nicely parallelizable, graphic processing units (GPUs) are perfectly suited for these algorithms. Here, we report on latest improvements to cuLGT, a CUDA-based software for lattice gauge fixing that evolved from the first GPU gauge fixing code presented in [1]. In its first version, cuLGT offered standalone applications for Landau, Coulomb and maximally Abelian gauge fixing in 3+1 dimensional SU(3) gauge theories using a combination of overrelaxation and simulated annealing [2]. One of the aims of cuLGT2 was to offer the possibility to integrate the gauge fixing routines in existing lattice QCD frameworks, like the MILC code [3]. In the following, we will restrict the discussion to Landau gauge and the overrelaxation algorithm. For a more complete treatment we refer to the original work [2].

An alternative GPU gauge fixing software using a Fourier accelerated steepest descent algorithm is available from the authors of [4].

2 Lattice Gauge Fixing

On the lattice, a link variable $U_\mu(x) \in \text{SU}(N_c)$ transforms with respect to gauge transformations $g(x) \in \text{SU}(N_c)$ as

$$U_\mu \rightarrow U_\mu^g = g(x)U_\mu(x)g^\dagger(x + \hat{\mu}).$$

The continuum Landau gauge condition,

$$\partial_\mu A_\mu(x) = 0,$$

translates on the lattice to the discrete derivative

$$\Delta(x) = \sum_\mu (A_\mu(x) - A_\mu(x - \hat{\mu})) = 0, \quad (1)$$

where the connection between the continuum gauge fields $A_\mu(x)$ and the lattice links is established by

$$A_\mu(x) = \frac{1}{2iag} [U_\mu(x) - U_\mu^\dagger(x)]_{\text{traceless}}.$$

In each local maximum of the Landau gauge fixing functional

$$F^U[g] = \frac{1}{N_d N_c V} \sum_x \sum_\mu \text{Re tr} [g(x)U_\mu(x)g^\dagger(x + \hat{\mu})] \quad (2)$$

the lattice Landau gauge condition (1) is satisfied. In the normalization of (2), $N_d = 4$ denotes the number of space-time dimensions and $V = N_s^3 N_t$ is the lattice volume. Instead of considering the complete functional (2), we rewrite it in a sum of local terms by factoring out the gauge transformation at lattice point x ,

$$F^U[g] = \frac{1}{2N_d N_c V} \sum_x \text{Re tr} [g(x)K(x)].$$

Then, we optimize

$$\text{Re tr} [g(x)K(x)] = \text{Re tr} \left[g(x) \sum_\mu [U_\mu(x) + U_\mu^\dagger(x - \hat{\mu})] \right]. \quad (3)$$

with respect to $g(x)$. All other (inactive) gauge transformations are set to the identity. The local functional (3) only depends on links that start or end at lattice site x .

The local maximum at each site can be found directly as

$$g(x) = K^\dagger(x) / \sqrt{\det K^\dagger(x)}$$

for the gauge group $\text{SU}(2)$. For $N_c > 2$ one iterates over the $\text{SU}(2)$ subgroups. To overcome the problem of critical slowing down, the authors of [5] proposed to apply an overrelaxation update by replacing $g(x)$ by $g^\omega(x)$ with $\omega \in [1, 2)$. Since only transformations at neighboring sites interfere, we can use a *checkerboard* layout and sweep first over the *black* and then over the *white* lattice sites. The algorithm is then iterated until the discrete gauge condition (1) is satisfied up to a given numerical precision.

3 GPU optimizations

Most GPU applications in lattice QCD are bound by the bandwidth of global device memory. Therefore, the highest focus should be on ideal memory usage. For an overview of optimization techniques for lattice QCD we refer to [6]. In the following, we will shortly summarize the optimizations that led to the performance of cuLGT1. In Sec. 4 we will report on the improved code cuLGT2.

3.1 Pre-cuLGT (first version)

For maximal throughput the memory access should be coalesced, i.e. consecutive threads should read from consecutive memory addresses. Therefore, we first reorder the lattice into its black and white sublattices according to the checkerboard layout. Within each sublattice we order data such that the site index runs faster than Lorentz and matrix indices.

In order to save bandwidth we do not load full $N_c \times N_c$ matrices from global memory, but only parts of it. Then, we use the properties of the gauge group to reconstruct the full matrix in registers/local memory. For the gauge group SU(3) we use a 12 parameter representation, i.e. the first 2 rows of the matrix.

With these optimizations we already get a remarkable speedup of a factor of ~ 30 over a single core CPU implementation¹ for the SU(3) overrelaxation code. The performance of 120 GFlops is of course far away from the theoretical peak performance of this GPU, however the correct measure of the utilization of the GPU is the achieved memory throughput. Therefore, on the r.h.s. of Fig. 1 we show the throughput in percent of the theoretical peak bandwidth. For this version of the code we only use 20% of the theoretical bandwidth².

3.2 cuLGT1

Register pressure turned out to be the main performance bottleneck in the first version of the code. There we used one thread to calculate the update of a site. A simple calculation shows that we would already need 144 registers for storing the 8 links that are involved in a site update (and additional registers are needed for temporary storage in the computation). Since the register limit of GPUs of the Fermi generation is 63 registers (32 bit) per kernel, a lot of data is spilled to the slow global memory. To relax the register pressure we introduced a 8-thread-per-site strategy in [2], where we keep one link (18 parameters) in each thread. The communication among these 8 threads (summation of links to get $K(x)$ and distribution of the result $g(x)$) is done via shared memory. With this optimization we increase performance by a factor of three, using more than 60% of the bandwidth. This version of the code is currently available on our website.

4 cuLGT2

With the development of cuLGT2 we wanted to solve several structural problems of cuLGT1: (a) the parameterization of links was hard-coded, switching to other parameterization would

¹We used our own reference CPU code which runs slightly faster than the publicly available MILC code [3]. However, for a *fair* comparison of CPU vs. GPU performance we would need a highly optimized multi-threaded CPU code.

²With the 12 parameter representation.

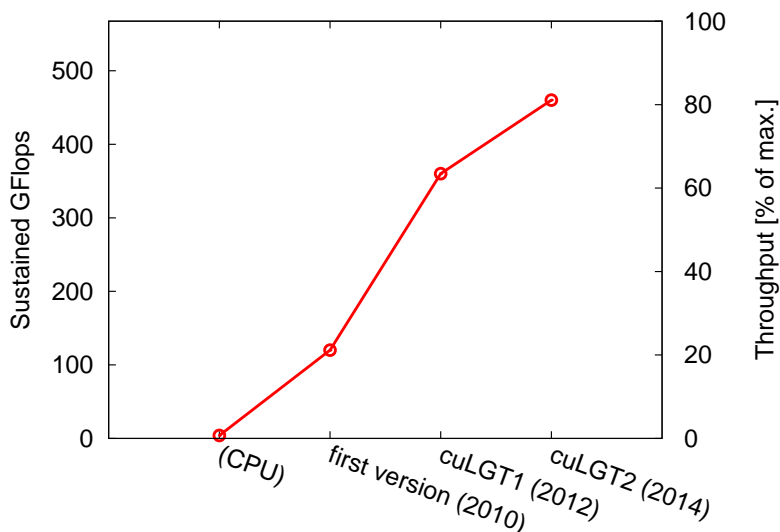


Figure 1: Evolution of the performance of cuLGT from the first version to cuLGT2 for the SU(3) Landau gauge overrelaxation code (32^4 lattice in single precision) on a GeForce GTX 580. The CPU performance is from a single core of an Intel Core i7-2600.

have needed a lot of code changes; (b) related to the former point, SU(2) and SU(3) implementations needed a lot of code duplication; (c) switching from the 8-threads-per-site strategy to 4 threads per site was not easily possible; (d) all these points prevented to implement a tool to automatically choose the optimal kernel settings for different GPUs, a technique that is already successfully used in the QUDA library [7].

To systematically solve these issues we decided to completely rewrite major parts of the code. In the following, we leave out most details of the implementation but focus only on the link management. This part might be useful for many other lattice GPU applications, since it allows developers to use high level constructs for writing GPU optimized code. A multi-GPU version of cuLGT2 is not yet available. We refer to cuLGT1 for lattice sizes that need multi-GPU.

4.1 Link management

Already in cuLGT1 we used two separate classes to represent a link in global memory `SU3<Link>` and local memory `SU3<Matrix>`. The former takes care of the memory pattern (details about available memory patterns in [2]) and allows to access a link by specifying the site and the Lorentz index. The data is stored in a linear `float` or `double` array of length $L = VN_d(2N_c^2)$, where $2N_c^2$ is the number of parameters of the $N_c \times N_c$ complex matrix. For using the 12 parameter representation one just reads/stores the first two rows of the matrix. Other representations where the parameters are not just a subset of the full matrix, like the minimal 8 parameter representation, are not provided. Changing the datatype of the global array was

also not possible³.

With cuLGT2, we decided to introduce an additional abstraction that easily allows changing how links are represented in memory. An implementation of a `ParameterizationType` defines the datatype and the number of elements. For transformations from one representation to another we define a mediator that overloads the assignment operator for the specific types. Links in global memory (`GlobalLink`) are now defined with two template parameters to specify the memory *pattern* and the *parameterization*. The `LocalLink` takes only the *parameterization* type as template parameter. Two examples for `ParameterizationTypes` for SU(3) are

```
class SU3Full                                class SU3Vector4
{
    typedef float TYPE;                      {
    const static int SIZE = 18;              typedef float4 TYPE;
                                           const static int SIZE = 3;
}                                           }
```

on the l.h.s. a 18 parameter representation with floats, usually used in `LocalLink`; on the r.h.s. a 12 parameter representation as three float4, usually used in `GlobalLink`. A (simplified) example code to perform a gauge transformation is

```
1 typedef GlobalLink<GPUPattern,SU3Vector4> GLOBALLINK;
2 typedef LocalLink<SU3Full> LOCALLINK;
3 void transformLink(Site s, int dir, LOCALLINK gLeft, LOCALLINK gRight)
4 {
5     GLOBALLINK global(s, dir);
6     LOCALLINK local;
7     local = global;
8     local = gLeft*local*gRight.hermitian();
9     global = local;
10 }
```

In line 1 and 2 the parameterizations for the `GlobalLink` and `LocalLink` are defined. Changing the gauge group to SU(2) would only require to set appropriate SU(2) parameterizations here. In line 7 a `GlobalLink` is assigned to a `LocalLink`. The full matrix is implicitly reconstructed. In line 8 the link is transformed. `LocalLink` overloads the multiplication operator and defines a function to compute the hermitian conjugate. The actual implementation of these operations is in the class of the `ParameterizationType`. In line 9 the modified link is written back to global memory, discarding the third line.

4.2 Performance

Although the primary design goal of cuLGT2 was not on performance improvements, we got a speedup compared to cuLGT1. The main improvement in Fig. 1 comes from the use of the 4-threads-per-site strategy instead of 8 threads per site. In Fig. 2 we compare the performance of the code on different GPUs. Only on the Tesla K20s 8-threads-per-site performs better. We do not yet know why this happens and why the result is that bad compared to the GTX Titan. Additional tuning is needed for the K20s.

³Using for example `float4/double2` instead of `float/double` would improve bandwidth utilization for memory accesses that cannot be coalesced, like access to links that are neighbors of the current site $U_\mu(x + \hat{\mu})$.

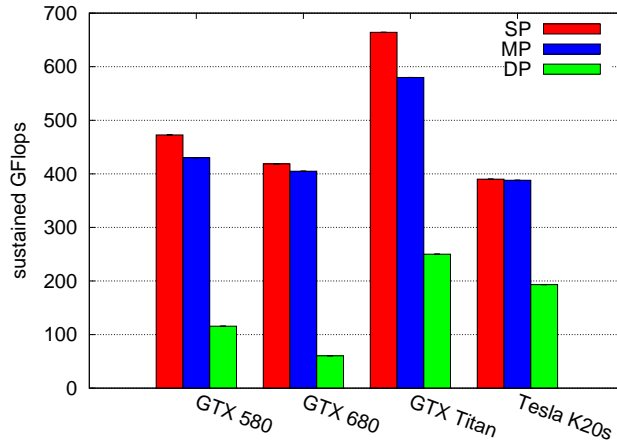


Figure 2: Performance of the cuLGT2 SU(3) Landau gauge overrelaxation code (32^4 lattice) on different GPUs in SP (left), mixed precision (middle) and DP (right)

5 Summary

With the development of cuLGT2 we successfully solved several design issues of cuLGT1. The gauge fixing software is now well modularized which allows us to run the gauge fixing routines from the MILC code. Additionally, the software automatically chooses the optimal kernel setup for different architectures at runtime by trying (a) 4 or 8 threads per site update, (b) different register limits by setting `--launchbounds()` (c) switching texture loads on or off. With the 4-threads-per-site strategy and the improved link management the performance of the code was remarkably improved.

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