ISU — Multigrid for computing propagators

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The Iteratively Smoothing Unigrid algorithm (ISU), a new multigrid method for computing propagators in Lattice Gauge Theory, is explained. The main idea is to compute good (i.e. smooth) interpolation operators in an iterative way. This method shows no critical slowing down for the 2-dimensional Laplace equation in an SU(2) gauge field. First results for the Dirac-operator are also shown.

1. The problem

The greatest obstacle for doing realistic (unquenched) simulations of lattice QCD is the large computer time required for the inversion of the Dirac-operator due to critical slowing down. Multigrid algorithms, which have been successful for the solution of differential equations describing ordered systems, have been studied for some time, but only with limited success.

In [1] we proposed the ideas of a new multigrid method to overcome these problems. This new algorithm, called Iteratively smoothing unigrid or ISU has been described in detail in [2]. Here we want to review it shortly and on general grounds and want to investigate its performance for the case of the 2-dimensional SU(2) bosonic and fermionic propagator equation.

2. The Unigrid

In this section, the basic principles of the multigrid method are presented from the unigrid point of view.

The two key observations are:

1. Standard relaxation algorithms (like Gauss-Seidel-relaxation) applied on a lattice with lattice constant $a$ are not efficient in reducing, but in smoothing the error on this scale. (The error is defined as the difference between the approximate and the exact solution.)

2. A function which is smooth on a length scale $a$ can be obtained by interpolation from a grid with lattice constant $\propto a$.

So the idea is to introduce, in addition to the fundamental lattice $\Lambda^0$ on which the problem is defined, auxiliary layers $\Lambda^j$ with lattice constants $a_j = L_j a_0$, where $L_j$, the blocking factor, is 2 or 3. The last of these lattices, $\Lambda^N$, consists of only one point. Points $x \in \Lambda^j$ can be identified with the corresponding points in $\Lambda^0$. We define blocks $[x]$ in $\Lambda^0$ with sidelength $2a_j - 1$ and the point $x$ in the center.

Let the fundamental equation be $D \xi = f$.

To an approximate solution $\tilde{\xi}$ corresponds an error $e = \xi - \tilde{\xi}$. We can cast the equation into the form $D e = r$, where $r = f - D \tilde{\xi}$ is the residual.

After relaxing on $\Lambda^0$, $e$ is smooth on scale $a_0$. It can therefore be obtained by interpolating it from a function $e^1$ on $\Lambda^1$ with the help of the interpolation operator $A^{[0,1]}$. $A^{[0,1]}$ maps functions on $\Lambda^j$ to functions on $\Lambda^0$, its adjoint $A^{[1,0]}$ blocks functions from $\Lambda^0$ to $\Lambda^j$. It has the property $A^{[1,0]}_z x = 0$ for $z \notin [x]$. So we get $e \approx A^{[1,0]} e^1$, resulting in the coarse grid equation

$$A^{[0,1]} D A^{[0,1]} e = A^{[0,1]} r \iff D^1 e^1 = r^1 \quad (1)$$

On this equation we relax again, thereby smoothing the error on scale $a_1$. We correct the approximation on the fundamental lattice $\xi \rightarrow \tilde{\xi} - A^{[0,1]} e^1$ and then we go to the next-coarser layer. (This is the difference to a true multigrid method: There one goes from $\Lambda^1$ directly to the next layer, without correcting first on the funda-
mental lattice. This is advantageous, because the work involved is less, but that the ISU-algorithm cannot work as a true multigrid, see [3]).

3. The need for smooth operators

The method described above can only work well if we know what is meant by the smoothness of the error after relaxation. It can be easily seen that in the context of lattice gauge theories, smoothness is not a priori defined, because no unique way to compare function values at different sites can be defined. Therefore we have to look for a new, appropriate definition. The following two definitions are in most cases equivalent.

Def. 1: A mode $\xi$ is smooth on scale $\lambda$ iff $\|L\xi\| \ll \xi$, $L$ in units $\lambda = 1$

Def. 2: A mode is smooth on scale $\lambda$ iff it is not efficiently reduced by relaxation on this scale.

That relaxation produces a smooth error not only according to the second, but also to the first definition, can be seen from the fact that usually the low-lying eigenmodes of $D$ are the bad-converging ones. (See [3] for a discussion of this and some caveats.)

To interpolate an error smooth in this sense, the interpolation operators $A^{[0,j]}$ have to be smooth themselves. So we have to find out how to calculate smooth interpolation operators. As the smoothest mode (according to def. 1) is the lowest eigenmode of $D$, it seems that we have to solve an equation as difficult as the one we started with to find the $A^{[0,j]}$.

4. The iteratively smoothing unigrid

But this is not true because of the following observation:

It is easier to calculate the shape of a mode which converges badly in a given iteration scheme than to reduce it directly with this scheme.

This can be seen from the following example: Imagine that $D$ only has one bad-converging mode $\psi$. Then we can compute this easily by trying to solve $D\xi = 0$, because in this case the approximate solution equals the error, which converges fast to a (small) multiple of $\psi$.

The second problem solving strategy is to solve our problem by reducing it to many similar problems which can be solved step by step.

The ISU algorithm for calculating good interpolation operators $A^{[0,j]}$ works as follows:

To calculate $A^{[0,j]}$ on a support $[x]$:

Solve $D_{[x]}A^{[0,j]}_x = \varepsilon_0 A^{[0,j]}_x$ via inverse iteration, using all interpolation operators on layers $\Lambda_k$ with $k < j$. (The righthandside could also be taken to be zero as in the above example, according to def. 2 of smoothness.) $|x|$ here means restriction to the block $[x]$, using e.g. Dirichlet boundary conditions.

The crucial point here is that the already calculated operators on the finer layers are used for the iteration, otherwise there would be many bad-converging modes and the calculation of $A^{[0,j]}$ would be slow.

5. Performance of ISU

We studied the performance of this algorithm in a two-dimensional SU(2) lattice gauge field, using the equation

$$(D - \varepsilon_0 + \delta m^2)\xi = f,$$  \hspace{1cm} \(2)$$

where $D$ was chosen to be the negative Laplace (bosonic case) or the negative squared staggered Dirac operator. $\varepsilon_0$ is the lowest eigenvalue of the operator which was subtracted to be able to tune criticality by changing the parameter $\delta m^2$. This subtraction is necessary for the Laplace operator (because its lowest eigenvalue can be large) and it eases the analysis of the critical behaviour also for the Dirac case.

We measured the asymptotic convergence rate $\tau$, i.e. the number of iterations needed to reduce the error by a factor $e$, where by an iteration we mean visiting each layer of the unigrid twice in a so-called V(1,1)-cycle (see [3]).

In the bosonic case we studied the convergence rate on grids of sizes $32^2$–$128^2$ at various values of the inverse coupling $\beta$. It was found, that $\tau$ was approximately 1, independent of the lattice size, $\beta$, and $\delta m^2$ (for small enough $\delta m^2$) which
Table 1
Convergence rate $\tau$ of the ISU-algorithm applied to the squared Dirac equation as a function of the grid length for physically scaled gauge fields.

| Grid size | 18$^2$ | 54$^2$ | 162$^2$ |
|-----------|--------|--------|---------|
| # runs    | 50     | 50     | 9       |
| $\beta$  | 1      | 9      | 81      |
| $\delta m^2$ | 0.002 | 0.002/9 | 0.002/81 |
| $\tau$    | 25.6 ± 0.9 | 6.67 ± 0.14 | 7.5 ± 0.8 |

means that the algorithm eliminates critical slowing down completely. Moreover it was found that the number of inverse iterations to calculate the smooth interpolation operators was six, again independent of the problem parameters, so critical slowing down does not enter through the backdoor. A detailed discussion of this result can be found in [2].

In applying the algorithm to fermions we used a block-factor of 3 instead of the more usual 2 to preserve the symmetry of the staggered grid also on the coarser layers [3]. The grid length therefore should be chosen as $L = 2 \cdot 3^N$, where $N$ is the number of layers. To improve convergence, we introduced an additional layer $\Lambda^{\text{add}}$, consisting of only four points, one for each pseudoflavour. This allows for more interpolation operators that cover a large part of the grid. (In the case of bosons, one could also use a block factor of three. There, the additional layer is not needed, because we found that even for this block factor $\tau$ was quite small and there was no critical slowing down.)

Table 1 shows preliminary results for the convergence rate for physically scaled gauge fields, i.e. for fields where $\beta \propto L^2$ and $\delta m^2 \propto L^{-2}$. The calculations were done on grids with grid size $18^2$–$162^2$ with $\beta = 1.0$ and $\delta m^2 = 2 \cdot 10^{-3}$ on the smallest lattice. Obviously there is no critical slowing down in this sense, which should be expected as the squared Dirac operator approaches the Laplacian in the continuum limit.

However, for small $\beta$ the convergence rates are bad (large absolute values) even on small lattices. The situation is much worse than for bosons, where $\tau$ was practically independent of all parameters.

6. Conclusions

The great success of the algorithm in case of the Laplace equation and the results obtained for the Dirac case pose three questions:

1. What is the crucial difference between the Laplacian and the Dirac operator, causing the one to converge much better than the other?

2. Can the algorithm be improved, perhaps by including insights gained from the answer to the first question?

3. How does the algorithm (or its improved version) behave in four dimensions?

At the moment we are studying mainly the first question. It seems that at least part of the answer lies in the shape of the low-lying eigenmodes of the Dirac-operator.

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