INSTRUCTIONS FOR TYPESETTING CAMERA-READY MANUSCRIPTS USING \TeX OR \LaTeX

FIRST AUTHOR
University Department, University Name, Address
City, State ZIP/Zone, Country

and

SECOND AUTHOR
Group, Laboratory, Address
City, State ZIP/Zone, Country

Received (received date)
Revised (revised date)

The abstract should summarize the context, content and conclusions of the paper in less than 200 words. It should not contain any references or displayed equations. Typeset the abstract in 8 pt Times roman with baselineskip of 10 pt, making an indentation of 1.5 pica on the left and right margins.

1. General Appearance

Contributions to the International Journal of Modern Physics C will be reproduced by photographing the author’s submitted typeset manuscript. It is therefore essential that the manuscript be in its final form, and of good appearance because it will be printed directly without any editing. The manuscript should also be clean and unfolded. The copy should be evenly printed on a high resolution printer (300 dots/inch or higher). If typographical errors cannot be avoided, use cut and paste methods to correct them. Smudged copy, pencil or ink text corrections will not be accepted. Do not use cellophane or transparent tape on the surface as this interferes with the picture taken by the publisher’s camera.

*For the title, try not to use more than 3 lines. Typeset the title in 10 pt Times roman, uppercase and boldface.
†Typeset names in 10 pt Times roman, uppercase. Use the footnote to indicate the present or permanent address of the author.
‡State completely without abbreviations, the affiliation and mailing address, including country. Typeset in 8 pt Times italic.
2. The Main Text

Contributions are to be in English. Authors are encouraged to have their contribution checked for grammar. American spelling should be used. Abbreviations are allowed but should be spelt out in full when first used. Integers ten and below are to be spelt out. Italicize foreign language phrases (e.g. Latin, French).

The text is to be typeset in 10 pt Times roman, single spaced with baselineskip of 13 pt. Text area (excluding running title) is 5 inches (30 picas) across and 7.8 inches (47 picas) deep. Final pagination and insertion of running titles will be done by the publisher. Number each page of the manuscript lightly at the bottom with a blue pencil. Reading copies of the paper can be numbered using any legible means (typewritten or handwritten).

3. Major Headings

Major headings should be typeset in boldface with the first letter of important words capitalized.

3.1. Sub-headings

Sub-headings should be typeset in boldface italic and capitalize the first letter of the first word only. Section number to be in boldface roman.

3.1.1. Sub-subheadings

Typeset sub-subheadings in medium face italic and capitalize the first letter of the first word only. Section numbers to be in roman.

3.2. Numbering and spacing

Sections, sub-sections and sub-subsections are numbered in Arabic. Use double spacing before all section headings, and single spacing after section headings. Flush left all paragraphs that follow after section headings.

3.3. Lists of items

Lists may be laid out with each item marked by a dot:

- item one,
- item two.

Items may also be numbered in lowercase roman numerals:

(i) item one
(ii) item two
   (a) Lists within lists can be numbered with lowercase roman letters,
   (b) second item.
4. Equations

Displayed equations should be numbered consecutively in each section, with the number set flush right and enclosed in parentheses.

\[
\mu(n, t) = \frac{\sum_{i=1}^{\infty} 1(d_i < t, N(d_i) = n)}{\int_{\sigma=0}^{t} 1(N(\sigma) = n) d\sigma}.
\]  

Equations should be referred to in abbreviated form, e.g. “Eq. (1)” or “(A.1)”. In multiple-line equations, the number should be given on the last line.

Displayed equations are to be centered on the page width. Standard English letters like x are to appear as x (italicized) in the text if they are used as mathematical symbols. Punctuation marks are used at the end of equations as if they appeared directly in the text.

**Theorem 1:** Theorems, lemmas, etc. are to be numbered consecutively in the paper. Use double spacing before and after theorems, lemmas, etc.

**Proof:** Proofs should end with \( \square \).

5. Illustrations and Photographs

Figures are to be inserted in the text nearest their first reference. Original India ink drawings of glossy prints are preferred. Please send one set of originals with copies. If the author requires the publisher to reduce the figures, ensure that the figures (including letterings and numbers) are large enough to be clearly seen after reduction. If photographs are to be used, only black and white ones are acceptable.

---

Fig. 1. Labeled tree \( T \).

Figures are to be sequentially numbered in Arabic numerals. The caption must be placed below the figure. Typeset in 8 pt Times roman with baselineskip of 10 pt. Use double spacing between a caption and the text that follows immediately.

Previously published material must be accompanied by written permission from the author and publisher.
6. Tables

Tables should be inserted in the text as close to the point of reference as possible. Some space should be left above and below the table.

Tables should be numbered sequentially in the text in Arabic numerals. Captions are to be centralized above the tables. Typeset tables and captions in 8 pt Times roman with baselineskip of 10 pt.

Table 1. Number of tests for WFF triple NA = 5, or NA = 8.

|   | 3  | 4  | 8  | 10  |
|---|----|----|----|-----|
| NP | 1200 | 2000 | 2500 | 3000 |
| NC | 2500 | 2700 | 16000 | 22000 |
| 8  | 3000 | 3400 | 22000 | 28000 |

If tables need to extend over to a second page, the continuation of the table should be preceded by a caption, e.g. “Table 2. (Continued)"

7. References

References in the text are to be numbered consecutively in Arabic numerals, in the order of first appearance. They are to be typed in superscripts after punctuation marks, e.g. “… in the statement.".

8. Footnotes

Footnotes should be numbered sequentially in superscript lowercase roman letters.

Acknowledgements

This section should come before the References. Funding information may also be included here.

References

References are to be listed in the order cited in the text. Use the style shown in the following examples. For journal names, use the standard abbreviations. Typeset references in 9 pt Times roman.

[1] J. Callaway, *Phys. Rev.* B35, 8723 (1987).
[2] M. Tinkham, *Group Theory and Quantum Mechanics* (McGraw-Hill, New York, 1964).
[3] T. Tel, in *Experimental Study and Characterization of Chaos*, ed. Hao Bailin (World Scientific, Singapore, 1990), p. 149.
[4] P. P. Edwards, in *Superconductivity and Applications — Proc. Taiwan Int. Symp. on Superconductivity*, ed. P. T. Wu *et al.* (World Scientific, Singapore, 1989), p. 29.
[5] W. J. Johnson, Ph.D. Thesis, Univ. of Wisconsin, Madison, 1968.

Footnotes should be typeset in 8 pt Times roman at the bottom of the page.
Appendix A

Appendices should be used only when absolutely necessary. They should come after the References. If there is more than one appendix, number them alphabetically. Number displayed equations occurring in the Appendix in this way, e.g. (A.1), (A.2), etc.

\[
\mu(n, t) = \frac{\sum_{i=1}^{\infty} 1(d_i < t, N(d_i) = n)}{\int_{\sigma=0}^{t} 1(N(\sigma) = n) d\sigma}.
\]  

(A.1)
We present a new multigrid method called neural multigrid which is based on joining multigrid ideas with concepts from neural nets. The main idea is to use the Greenbaum criterion as a cost functional for the neural net. The algorithm is able to learn efficient interpolation operators in the case of the ordered Laplace equation with only a very small critical slowing down and with a surprisingly small amount of work comparable to that of a Conjugate Gradient solver.

In the case of the two-dimensional Laplace equation with SU(2) gauge fields at $\beta = 0$ the learning exhibits critical slowing down with an exponent of about $z \approx 0.4$. The algorithm is able to find quite good interpolation operators in this case as well. Thereby it is proven that a practical true multigrid algorithm exists even for a gauge theory. An improved algorithm using dynamical blocks that will hopefully overcome the critical slowing down completely is sketched.

Keywords: Discretized differential equations, multigrid, neural nets, disordered systems, lattice gauge theory

1. Introduction

Multigrid methods are among the most successful strategies for solving discretized differential equations. In the presence of disorder, which is the case of most interest to contemporary physics, the development of methods that are able to deal with the lost translational invariance of the system has proven extremely difficult. As an example we may look at the efforts to find a multigrid solver for the Dirac equation in Lattice Gauge Theory, reviewed in\cite{1}. Up to now, no true multigrid algorithm has been found that is able to deal with this problem as efficiently as we would like, although there is a unigrid method called ISU that has been proven to work in two dimensions\cite{1}.

The development of the ISU algorithm has been triggered by an attempt to connect multiscale ideas with the method of neural nets\cite{3}. A more direct combination of multigrid and neural net methods was based on the idea to learn the shapes of slow-converging modes by a standard back-propagation scheme, using the known errors of test problems as targets. This, however, was shown to be not feasible\cite{13}. The main reason was that the cost functional possessed only a very narrow mini-
mum, which was difficult to find by the neural net whenever the criticality of the problem operator (i.e. its condition number) was large.

In this work we retain the idea of using test problems to do the learning, but we do not try to learn them as in a pattern recognition neural network. Instead of this, we borrow ideas from the ISU algorithm\textsuperscript{1} and the principle of indirect elimination\textsuperscript{2}.

2. The problem

Consider a linear operator $\mathbf{D}$ which may arise from a discretized differential equation defined on a cubic lattice $\Lambda^0$.\textsuperscript{Here and in the following we assume $\mathbf{D}$ to be positive definite, if it were not, we could use the operator $\mathbf{D}^* \mathbf{D}$ instead. The general form of the equation to be solved is then

$$\mathbf{D} \xi = f,$$

(1)

It is well known that standard solvers like Conjugate Gradient or Overrelaxation show the phenomenon of critical slowing down: The number of iterations needed to solve the equation with a given precision scales with some power of the condition number (quotient of the largest and smallest eigenvalue).

At each time-step, any iterative method will yield an approximate solution $\tilde{\xi}$. We introduce two important quantities: the error $e = \xi - \tilde{\xi}$ which is the difference between the true and the actual solution and is of course not known, and the residual $r = f - \mathbf{D} \tilde{\xi}$, the difference between the true and the actual righthandside. With these definitions we can recast the fundamental equation (1) as

$$\mathbf{D} e = r,$$

(2)

called the error equation.

For a linear method, we can also introduce the iteration matrix $\mathbf{S}$ which tells us what the new error after the next iteration step will be, given the old one:

$$e^{\text{new}} = \mathbf{S} e^{\text{old}}.$$

(3)

3. The Neural Multigrid

Although our method is motivated by ideas borrowed from neural network methods, a thorough understanding of these methods is not necessary. A good introductory text is\textsuperscript{10}. For introductions to multigrid see\textsuperscript{5,6,9}.

The basic setup of a multigrid algorithm uses auxiliary lattices, also called block lattices or coarse grids, $\Lambda^1, \Lambda^2, \ldots, \Lambda^N$ with lattice spacings $a_j = L_j a_0$, where $L_b$ is the blocking factor and is usually chosen to be 2. The last lattice $\Lambda^N$ should contain few enough points that a direct solution of any equation living on this lattice is easy.

\textsuperscript{a}It is not necessary to restrict our attention to the case of a cubic lattice, but it eases the implementation of the method.
Let $H^j$ be the space of functions on lattice $\Lambda^j$. Then we introduce grid transfer operators:

the interpolation operators: $A^k : H^{k+1} \rightarrow H^k$ and

the restriction operators: $C^k : H^k \rightarrow H^{k+1}$,

with $k < N$. So operators $A^k$ interpolate from a coarser to a finer grid, whereas the restriction operators do the reverse. For reasons of efficiency these operators are not allowed to interpolate from one block grid point to all of the fine grid: if we identify a block grid point $x$ with its corresponding fine grid point $z$ we must require $A^k(z, x) = 0$ unless $x$ lies near $z$. We will always choose the operators to be adjoints of each other: $C^k = A^k^*$. We also recursively define effective operators

$$D^k = C^k - 1D^{k-1}A^{k-1},$$

of course setting $D^0 = D$ to stop the recursion.

Multigrid methods are based on the observation that standard relaxation algorithms usually smoothen the error, or in more general terms, project onto the lower half of the eigenspectrum of the problem operator $D^0$. If we can find interpolation operators $A^0$ such that the smooth error lies within their range, we can write $e^0 \approx A^0e^1$. Inserting this into the error equation (2) we find

$$D^0 A^0 e^1 = r^0$$

$$C^0 D^0 A^0 e^1 = C^0 r^0$$

$$D^1 e^1 = r^1,$$

involving only quantities on the block lattice. Solving this equation and interpolating back yields a good estimator for the error $e^0$. The block-equation (5) can be solved recursively by going to a still coarser grid, until we reach the coarsest layer $\Lambda^N$ where the equation can be solved directly.

After this review of multigrid methods let us now set up the neural multigrid. The basic fact we are using is the Greenbaum criterion, which up to now has been considered to have no practical use at all. It states that optimal convergence of the multigrid is achieved when the interpolation operators are able to represent all the modes of the system that are slowly converging under the used relaxation process. In other words, all the highest eigenmodes of the iteration matrix of the relaxation process have to lie within the range of the interpolation operators. Stated like this it is clear why the practical value of this principle is small: How should we know all of the bad-converging modes of the system?

To learn these modes we are going to use test problems: A test problem is a problem with a known solution, chosen such that the initial error is a random function on the lattice. This can be done by drawing the exact solution $\xi$ from a random distribution, calculating the test problem’s righthandside $f = D\xi$ and starting with the initial guess $\tilde{\xi} = 0$.

A first idea to exploit the criterion uses the fact that indeed we have a good projector onto the bad-converging modes, namely the relaxation process itself. Therefore it would be possible to start with a test problem, do some relaxations and
Another Look at Neural Multigrid

thereby project the initial error onto the space of the slow-converging modes. This error could then be learned (in some way) by the neural multigrid.

Of course this method is doomed to fail: To exhaust the complete space of the slow modes would take a very long time because the projection on the worst modes will only be efficient after many relaxation sweeps. This means that the projection method itself suffers from critical slowing down, and therefore our neural multigrid will as well.

Nevertheless, our new method is based on this idea, but with another ingredient, which is similar to the spirit of ISU: After a few relaxation steps, the remaining error is something that should definitely be learned. So we adapt our interpolation operators to this error (the details will be explained later on), and then use the newly learned interpolation operators to further reduce the error. To do so, we can make a coarse-grid correction step. (For the time being, think of the method as a two-grid-method, i.e. \( N = 1 \).) This then efficiently removes all those error components already learned. We then relax again and start the learning process anew (of course using everything we have already learned).

It is easy to see why this avoids the pitfall described above: After the first relaxation step the error will contain contributions from all slow modes. Some of these will be learned by the multigrid and are therefore removed. In this way we successively project out everything that is not yet learned and then learn it. After each learning step, we measure the convergence rate of the algorithm as it stands now by solving another test problem. If this is sufficient (for instance, if the error is reduced by a factor of 2 during each multigrid cycle), we stop the learning procedure, otherwise we continue.

It may happen that one coarse-grid correction step is not enough to project the error onto the nullspace of the interpolation operators. In this case we may use the error \( e_M \) of the measurement iteration for the next learning step by setting \( f = D e_M \). This was the method actually used to obtain the results shown below.

4. The learning process

Let us now look at the method in greater detail: How is the learning actually done?

The first thing in setting up a neural network is to decide on a cost functional that decides how good a certain network configuration is. As we want to have the error after relaxation within the range of the interpolation operators, we choose as functional

\[
E = \frac{\| A \delta e - e \|^2}{\| e \|^2},
\]

where \( A \) is the interpolation operator, \( e \) is the actual error and \( \delta e \) is chosen such as to minimize \( E \) with the given interpolation operators, at least approximately. \( \delta e \) is the coarse-grid correction we would get using these interpolation operators, so it is a function living on the coarse grid. With \( x \) being a coarse grid point and \( z \) a fine
Another Look at Neural Multigrid

grid point, we can rewrite $E$ using indices as

$$E = \frac{\sum_z \left( \sum_x A(z, x) \delta e(x) - e(z) \right)^2}{\sum_z e(z)^2}.$$  \hspace{1cm} (10)

There are two possibilities to use this cost functional: The standard way in neural networks would be to calculate the derivatives $\partial E/\partial A(z, x)$ and do an adjustment step in direction of this gradient, perhaps also including some momentum term.[4]

However, we can do better than this: Remembering that our interpolation operators are localized objects, we see that at each point the derivative only depends on very few of the interpolation operators. We can therefore minimize $E$ exactly at each point so that the actual error lies within the range of the interpolation operators. To do so, we require $\partial E/\partial A \equiv 0$ at each point. This is possible only because the space of interpolation operators is larger than the space of fine grid functions, as most of the fine grid points are covered by more than one interpolation operator. In fact, the system of equations $\partial E/\partial A \equiv 0$ is under-determined because of this. This is an advantage as we can adjust the interpolation operators and still retain some memory of their old values.

To describe the rules of the learning, let us define the difference vector $d(z) = \sum_x A(z, x) \delta e(x) - e(z)$, which is nothing but the error after the correction step using $\delta e$. By $\delta A(z, x)$ we denote the change in $A$ at the specified point. The condition to be fulfilled is therefore that $d(z)$ would be zero after the change of $A$:

$$\sum_x \left( A(z, x) + \delta A(z, x) \right) \delta e(x) - e(z) \equiv 0.$$  \hspace{1cm} (11)

As this system of equations is under-determined, we may add another requirement. In order to keep some memory of already learned things, we require that $\sum_{x, z} \delta A(z, x)^2 \equiv \min$, so we look for that choice of $A$ that is closest to the old $A$.

To solve these equations we can use the method of Lagrangian multipliers (minimizing the change in $A$ and using eq. (11) as a constraint) and we find

$$\delta A(z, x) = -\frac{d(z) \delta e(x)}{\sum_{x', x' \ni z} \delta e(x')}.$$  \hspace{1cm} (12)

Here the condition $x' \ni z$ means that we have to use all those points $x'$ from which the interpolation operator can reach the point $z$.

Finally, let us remark on the choice of $\delta e$: The obvious method to determine it would be to use a full coarse-grid-correction step. A somewhat simpler (and cheaper) choice is to choose $\delta e$ such that the error is put to zero at those fine grid points only reached by one interpolation operator, i.e. in the center of each block. This should result in a good approximation of the optimal choice of $\delta e$ and is much cheaper. Up to now, this method has been used.
5. The true multigrid

For a true multigrid, all we have to do is to use the algorithm above recursively. Whenever a coarse-grid-correction is required, we try to solve the coarse grid equation, monitoring the convergence. If the convergence is not good enough, we set up a test problem on the coarse layer, learn good interpolation operators on this layer and then solve the coarse grid equation again.

This looks like a very expensive method, for the average number of learning cycles required on a certain layer will quickly blow up the coarser the layer is. If we need only two learning steps in each learning process the method will proceed through the multigrid in a W-cycle fashion — more learning steps are analogous to higher cycles. In two dimensions, the maximal cycle index allowed is four, so we will quickly reach a limiting point where learning becomes extremely slow and has some kind of critical slowing down.

Two facts oppose this tendency for the process to get slow: First of all, as long as the interpolation operators are not yet very good, the coarse grid equation will not be as critical as the fine grid equation, so solving it is easier. Secondly, as the changes on each layer are gradual, not every change on a fine layer will need adaptations on coarser layers.

Of course, a definite answer can only be found by putting the method to the test.

6. Possible improvements

6.1. Adding an indirect elimination

A very simple improvement that can be added to the algorithm is to introduce an update based on the principle of indirect elimination: If the convergence rate is not satisfactory, we store the error after a measurement and do a line search in the direction of this error vector before each multigrid cycle. As the error after the measurement corresponds (at least approximately) to the worst-converging mode of the algorithm, the line search will take care of this mode, so that it will not contribute to the error in the following multigrid steps. A thorough explanation of the principle of indirect elimination can be found in 2.

6.2. Adding a memory

Another possibility is to store some of the errors learned and to relearn them in later learning cycles. As we exactly minimize the cost function in each step, we may forget some of the error shapes learned earlier. If we store these errors, we can use them again. In this way we attempt to find interpolation operators that are able to deal with all the learned error shapes. It is well-known from the neural net context that a shape once learned might be forgotten later on if it is not shown again to the network. To be more precise, what we add to the algorithm are the following steps:
Instead of the simple adaptation step we have

\begin{verbatim}
do nrOfMemorySteps times:
    Adapt to the actual error
    Adapt to all memorized errors
    Adapt to the actual error again
\end{verbatim}

In practice, we usually choose to do three memory steps. We store only those errors for later relearning whose learning has reduced the convergence time appreciably.

7. Results for the ordered case

As a first test we investigated the neural multigrid for the standard Laplace equation in two dimensions on a square lattice. We use periodic boundary conditions and add a small mass term:

\begin{equation}
(\Delta + m^2) \xi = f.
\end{equation}

It is well known that in this case a standard multigrid method will exhibit excellent convergence properties, reducing the error at least by a factor of ten in each multigrid cycle.

We studied the behaviour of our neural multigrid on lattices of size $16^2$ up to $64^2$. The coarsest layer was always chosen to have a size of $2^2$, so that the scaling behaviour of the algorithm could be studied. Remember that this is one of the key questions for this method: How much do the additional learning steps on the coarser layers affect the overall work done by the algorithm?

For a simple test case in one dimension it was found that the situation is not favorable: The larger the lattice became, the greater was the amount of work needed to learn good interpolation operators. We estimated a critical exponent of 0.5. However, the larger the dimension, the smaller is the relative size of the block lattices compared to the finest lattice, so in higher dimensions the situation might get better.

Figure 1 shows the work needed to learn interpolation operators that achieve the textbook efficiency of a reduction factor of at least 10 in each multigrid cycle for the two-dimensional case. The work was measured in elementary vector operations, i.e. each vector addition, multiplication on the finest layer etc. counts as one work unit, a vector operation on the first block layer as $1/4$ work units and so on. For each set of parameters ten runs have been made. (Note that although the problem operator is always the same, the righthandside and the randomly chosen start vectors differ on each run.)

We can see two things: The number of work units needed does not grow with the lattice size. This is an encouraging result because it means that the recursive structure of the method does not lead to an impractical algorithm.

On the other hand we can see that the needed work does increase with the criticality of the problem. For mass values smaller than $10^{-4}$ the work grows appreciably when we lower the mass further. We see that the work needed at masses
Figure 1: Number of Work units (elementary vector operations; see text) needed by the neural multigrid to learn interpolation operators with a reduction rate of smaller than 0.1 and to solve the simple Laplace equation. For each data point, ten runs were made. The work does not depend on the lattice size, but for very small eigenvalues the needed work increases. (At $10^{-6}$ one of the runs on the $16^2$-lattice did not converge, this was not taken into account here, see text.) Note the offset of the y-axis.
Another Look at Neural Multigrid

Figure 2: Reduction factor \( \rho \) achieved by the neural multigrid after one learning step on the finest lattice has been completed. Again there is no dependence on the lattice size, but for very small mass values of the Laplace equation the reduction factor is gets large.

\( 10^{-5} \) is approximately twice that we need at mass \( 10^{-2} \); out of this we would estimate a critical exponent of 0.2. (The critical exponent \( z \) for fixed lattice size is given by \( \text{Work needed} \propto \kappa^{z/2} \), where \( \kappa \) is the condition number.) This is a fairly small value (e.g. when compared to the value for Conjugate Gradient algorithms with \( z = 1 \)). Of course, with the present data we cannot exclude that the work needed will grow faster when we decrease the mass even further.

At a mass value of \( 10^{-6} \) on a \( 16^2 \)-lattice, the neural multigrid did not reach the required convergence rate within 20 learning cycles in one of the ten runs. However, it did achieve a reduction factor of 7 within a few iterations. This run has not been taken into account in the picture, but it shows again that the algorithm has greater difficulties at very small eigenvalues.

We can also look at the reduction rate \( \rho \) that is achieved after the first learning step on the finest layer is finished, see figure 2. Again we see that for masses of \( 10^{-4} \) and larger the results are very good and textbook efficiency is usually achieved; for smaller mass values the convergence deteriorates.

Although the results are not too bad, we can overcome this deterioration by adding an improvement as explained in section 6.1. The application of the principle of indirect elimination will eliminate the contribution from the lowest eigenmode of the problem operator, which is the one causing the problems here. After adding such an updating step the convergence stays constant regardless of the mass value. Note, however, that this is only possible because the number of low-lying eigenmodes is small in the case of the Laplace equation.
We believe that the results shown in this section are quite encouraging: There is no dependence of the work needed on the lattice size. Furthermore, except for very high criticality the absolute number of work units is not too high. For comparison, a Conjugate Gradient algorithm needs about 3700 work units to solve the equation with the desired accuracy on the $64^2$-lattice at a mass value of $10^{-4}$. (Note that the work for the final solution of the equation is included in figure 1.) This is about a factor of two smaller that the work needed by the neural multigrid; however we have not tuned the parameters to minimize the work; for instance the number of multigrid sweeps done in each measurement has been chosen to be 20, which is quite large. In addition, during the program runs several test measurements of errors, residuals etc. are done that are not strictly necessary. Therefore we believe that the neural multigrid still has a great potential for improvements. The real test is of course its behaviour in the case of disordered problems.

8. Lattice Gauge Theory

8.1. The Problem

As an example for a disordered system we consider the propagator equation for a bosonic particle in an SU(2)-gauge field background. The covariant Laplace-operator in stencil-notation is

$$\Delta(z) = \begin{bmatrix} 0 & U_{z,2} & 0 \\ U_{z,-1} & 4 & U_{z,1} \\ 0 & U_{z,-2} & 0 \end{bmatrix},$$

with $U_{z,\mu} \in \text{SU}(2)$. The second index denotes the direction of the coupling to the neighbour. The link matrices $U_{z,\mu}$ fulfill $U_{z,-\mu} = U_{z,\mu}^*$. They are distributed according to the Wilson action

$$S_W = \frac{\beta}{4} \sum_P \text{Re tr} \ (1 - U_P).$$

Here $\beta = 4/g^2$ is the inverse coupling and the sum is over all Plaquettes in the lattice. $U_P$ denotes the parallel transport around a Plaquette. This distribution leads to a correlation between the gauge field matrices with finite correlation length $\chi$ for finite $\beta$. The case $\beta = 0$ corresponds to a completely random choice of the matrices ($\chi = 0$), for $\beta = \infty$ all matrices are 1 ($\chi = \infty$). In this sense, $\beta$ is a disorder parameter, the smaller $\beta$ the shorter the correlation length and the larger the disorder.

Here we are only interested in the behaviour of our algorithm for a disordered system and so we will choose in the following $\beta = 0$, which gives the greatest disorder possible.

As it stands, however, the equation is not critical: The lowest eigenvalue will be quite large (of the order of 0.5). To get a disordered critical problem we first
Figure 3: Number of Work units needed by the neural multigrid to learn interpolation operators with a reduction rate of smaller than 0.6 and to solve the SU(2) Laplace equation. For each data point, ten runs were made, except for the $32^2$ and $64^2$ lattices at $\delta m^2 = 10^{-4}$, where 20 and 15 runs were done.

calculate the lowest eigenvalue and then subtract it from the diagonal part of the operator. This allows us to tune criticality and thereby to measure the convergence behaviour accurately. Note that this destroys the diagonal dominance of the operator and makes the problem quite difficult for a multigrid method.

8.2. Results

Trying the neural multigrid on the described problem, we found quickly that it was not possible to achieve the desired textbook efficiency of $\rho = 0.1$. A more realistic goal seemed to require the neural multigrid to reach a $\rho < 0.6$, which means that for the same error reduction we need about four times the work. But if this could be reached regardless of criticality and lattice size, the algorithm would still be very efficient.

To improve the convergence, we introduced the improvements described in section 6. However, as a look at fig. 3 shows, the work needed to learn good interpolation operators that achieve the desired reduction rate grows with the criticality and at first also with the lattice size. The growth with the lattice size stops as soon as the $32^2$-lattice is reached, so for large enough lattices there seems to be no critical slowing down here. For the growth with the criticality the exponent can be estimated roughly to be about $z \approx 0.4$. Although this is not too bad, the absolute number of work units is quite large; about 15 times larger than that needed by a Conjugate Gradient algorithm.
These results are somewhat disappointing. As it stands, the algorithm is not as efficient as we hoped for. Nevertheless, we have achieved an important result: The algorithm was able to find interpolation operators that allow for multigrid cycles with $\rho < 0.6$ in almost all cases. This means that we have shown numerically that there exists a practical true multigrid algorithm for a two-dimensional bosonic gauge theory without critical slowing down. Up to now it was only known that idealized multigrid algorithms (in four dimensions) were able to eliminate critical slowing down, but these used non-local interpolation operators. The ISU algorithm also eliminates critical slowing down for our test problem, but being a unigrid the work it needs grows as $\ln^2(\text{Volume})$. By investigating the interpolation operators found by the neural multigrid more closely we might find valuable informations about how good interpolation operators should look like. The same can also be tried for the case of greater interest, namely the four-dimensional Dirac equation.

8.3. Overcoming the difficulties

Is it possible to overcome the described difficulties? To answer this, we have to investigate the reason for the problems with the gauge theory. A first hint is that most of the work was done on the coarser layers. This means that as a twogrid, our algorithm would have (nearly) no critical slowing down. Are the coarser layers more problematic than the finest one?

Indeed they are. As the interpolation operators are not simple linear functions, the effective operator $D^k$ has strongly fluctuating couplings and a fluctuating diagonal term as well. A simple look at the operators shows that after two blocking steps the coupling strengths may vary by a factor of ten or more. It is well known that for couplings with such strong fluctuations a simple blocking scheme with square blocks will not be efficient.

In order to overcome this difficulty, an algorithm to determine good shapes for the supports of the interpolation operators is needed. Such an algorithm was developed as a part of the Algebraic Multigrid and could be used as an ingredient to our neural multigrid. This algorithm chooses those points as block-centers that have many strong connections to other points of the lattice and is quite efficient.

A preliminary study to confirm this picture was also done: We used the scalar Laplace equation with a site-dependent mass term. At low criticality, the neural multigrid again exhibited critical slowing down when the mass term was strongly fluctuating. A study of the errors showed that indeed these are the points where the error is not properly reduced. This problem was partly alleviated by shifting the lattice such that the points with the weakest connections were not chosen as block-centers, however some critical slowing down still remained.

So it is probable that using dynamically chosen blocks the algorithm would perform much better, perhaps even without critical slowing down.

9. Conclusions
We have presented a new multigrid method called neural multigrid which is based on joining multigrid ideas with concepts from neural nets. The algorithm is able to learn efficient interpolation operators in the case of the ordered Laplace equation nearly without critical slowing down and with a surprisingly small amount of work comparable to that of a Conjugate Gradient solver.

In the case of a disordered system (the Laplace equation with SU(2) gauge fields) the learning exhibited critical slowing down with an exponent of about $z \approx 0.4$ and the algorithm was able to find good interpolation operators in this case as well. Finally it was shown that the remaining critical slowing down of the algorithm might be overcome by choosing the supports of the interpolation operators dynamically.

Acknowledgments

I wish to thank Daniel Lübbert for rekindling my interest in neural multigrid. Financial support by Deutsche Forschungsgemeinschaft is gratefully acknowledged.

References

1. M. Bäker, *Int. J. Mod. Phys. C*, 85 (1995)
   M. Bäker, *A Multiscale View of Propagators in Gauge Fields*, Ph. D. Thesis, Hamburg, DESY 95-134, 1995
2. M. Bäker, *Int. J. Mod. Phys. C7*, 503 (1996)
3. M. Bäker, G. Mack, M. Speh, *Nucl. Phys. B30* (proc. Supp.), 269 (1993)
   M. Bäker, T. Kalkreuter, G. Mack, M. Speh, *Int. J. Mod. Phys. C4*, 239 (1993)
4. A. Brandt, *Nucl. Phys. B 26*, (Proc.Suppl.), 137 (1992)
5. A. Brandt, *Multigrid Techniques: 1984 guide with applications to Fluid Dynamics*, GMD-Studie Nr. 85
6. W. L. Briggs, *A Multigrid Tutorial*, SIAM, Philadelphia 1987
7. M. Creutz, *Quarks, Gluons, and Lattices*, Cambridge University Press, Cambridge 1983
8. A. Greenbaum, *SIAM J. Numer. Anal. 21*, 657, 1984
9. W. Hackbusch, *Multigrid Methods and Applications*, Springer Series in Computational Mathematics 4, 1985
10. J. Hertz, A. Krogh, R. Palmer, *Introduction to the theory of neural computation*, Santa Fe Institute lecture notes, Addison Wesley, 1992
11. T. Kalkreuter, *Phys. Rev. D 48*, 1993, 1925
    T. Kalkreuter, *Int. J. Mod. Phys. C 5*, 1994, 629
12. T. Kalkreuter, *Multigrid Methods for Propagators in Lattice Gauge Theory*, Invited lecture at Modelling 94, Prague, Czech Republic, J. Comp. Appl. Math. (Proc. Suppl.)
13. B. Mikska, *Feasibility Study of a recursive neural Multigrid Method for disordered Systems*, unpublished
    reviewed in: D. Lübbert, *Anwendungen systemtheoretischer Verallgemeinerungen von Algorithmen der Gitterfeldtheorie*, Diploma Thesis, Hamburg 1996
14. J. Ruge, K. Stüben, in S. McCormick, *Multigrid Methods, Frontiers in Applied Mathematics Vol. 5*, SIAM, Philadelphia 1987
15. R. Varga, *Matrix Iterative Analysis*, Prentice Hall, Englewood Cliffs, NJ, 1962
16. K. G. Wilson, *Phys. Rev. D 10*, (1974), 2445
17. D. Young, *Iterative Solutions of Large Linear Systems*, Academic Press, New York 1971