Layer-Parallel Training of Deep Residual Neural Networks

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Abstract

Residual neural networks (ResNets) are a promising class of deep neural networks that have shown excellent performance for a number of learning tasks, e.g., image classification and recognition. Mathematically, ResNet architectures can be interpreted as forward Euler discretizations of a nonlinear initial value problem whose time-dependent control variables represent the weights of the neural network. Hence, training a ResNet can be cast as an optimal control problem of the associated dynamical system. For similar time-dependent optimal control problems arising in engineering applications, parallel-in-time methods have shown notable improvements in scalability. This paper demonstrates the use of those techniques for efficient and effective training of ResNets. The proposed algorithms replace the classical (sequential) forward and backward propagation through the network layers by a parallel nonlinear multigrid iteration applied to the layer domain. This adds a new dimension of parallelism across layers that is attractive when training very deep networks. From this basic idea, we derive multiple layer-parallel methods. The most efficient version employs a simultaneous optimization approach where updates to the network parameters are based on inexact gradient information in order to speed up the training process. Using numerical examples from supervised classification, we demonstrate that our approach achieves similar training performance to traditional methods, but enables layer-parallelism and thus provides speedup over layer-serial methods through greater concurrency.

1 Introduction

One of the most promising areas in artificial intelligence is deep learning, a form of machine learning that uses neural networks containing many hidden layers [4, 42]. Even though neural networks date

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back at least to the 1950’s [46], recent advances in computer hardware as well as the availability of ever larger data sets have enabled and fueled the success of modern machine learning techniques. Since then, deep neural networks (DNNs), and in particular deep residual networks (ResNets) [34], have been breaking human records in various contests and are now central to technology such as image recognition [36, 41, 42] and natural language processing [6, 15, 39].

The abstract goal of machine learning is to model a function $f : \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^m$ and train its parameter $\theta \in \mathbb{R}^p$ such that

$$f(y, \theta) \approx c$$

(1.1)

for input-output pairs $(y, c)$ from a certain data set $\mathcal{Y} \times \mathcal{C}$. Depending on the nature of inputs and outputs, the task can be regression or classification. When outputs are available for all samples, parts of the samples, or are not available, this formulation describes supervised, semi-supervised, and unsupervised learning, respectively. The function $f$ can be thought of as an interpolation or approximation function.

In deep learning, the function $f$ includes a DNN that aims at transforming the input data. In the case of feed forward networks, this process is called forward propagation and for an $N$-layer neural network one starts with $u^0 = y$ and proceeds with $u^{n+1} = \Phi(u^n, \theta^n)$ for all $n = 0, 1, \ldots, N - 1$, which propagates the input data through all layers of the network. Here, the vector of parameters $\theta \in \mathbb{R}^p$ is partitioned into parameters for each layer, $\theta^0, \theta^1, \ldots, \theta^{N-1}$. In this paper, we consider a special type of forward propagation given by ResNets [34], for which the forward propagation reads

$$u^{n+1} = u^n + hF(u^n, \theta^n),$$

(1.2)

where $h > 0$ is a constant and the layer function $F$ consists of relatively simple operations, such as affine linear mappings parameterized by the parameters $\theta^n$ and nonlinear element-wise activation functions. While we restrict the discussion to feed-forward networks for supervised classification, the layer-parallel integration can be extended to some recurrent learning tasks and, when the output data is replaced with a reward function, reinforcement learning (for general introductions to this field see, e.g., [22, 2, 28]).

The training problem consists of finding the parameters $\theta^n$ such that (1.1) is satisfied for elements from a training data set but also holds for previously unseen data from a validation data set which has not been used during training. The former objective is commonly modeled as an expected loss and optimization techniques are used to find the parameters that minimize the loss. Using networks with a sufficient number of layers and parameters and adequate minimization techniques, it is typically possible to obtain a solution with an arbitrarily low expected loss. However, similar to polynomial interpolation, this strategy may result in overfitting and minimizers may perform poorly on data not used during the training, in other words, the network fails to generalize. Designing learning strategies that ensure generalization is a subject of current research.

Despite the rapid methodological developments, compute times for the training of state-of-the-art DNNs can still be prohibitive, measured in the order of hours or days, involving hundreds or even thousands of layers and millions or billions of network parameters [16, 40]. There is thus a great interest in increasing parallelism to reduce training runtimes. Common approaches involve data- and model-parallelism. Data-parallelism refers to the idea of distributing elements of the training data set onto multiple compute units. Synchronous and asynchronous data-parallel training algorithms have been developed to coordinate the network parameter updates [37, 1]. In contrast, model-parallelism refers to partitioning the different layers of the network and its parameters to different compute units. Model parallelism has traditionally been used when the network dimension
exceeds available memory of a single compute unit. Often, a combination of both approaches is employed [33, 16]. However, none of the above approaches to parallelism tackle the scalability barrier created by the serial propagation of data elements through the network layers itself. In either above approach, each subsequent layer can process information only after the previous layer has finished its computation. As a result, training runtimes scale linearly with the number of layers. As current state-of-the-art networks tend to increase complexity by adding more and more layers (see, e.g., the ResNet-1001 with 1001 layers and 10.2 million weights in [35]), the serial layer propagation creates a serious bottleneck for fast and scalable training algorithms that leverage modern HPC architectures.

In this paper, we address the above scalability barrier by introducing concurrency across the network layers. To this end, we replace the serial data propagation through the network by a nonlinear multigrid method that treats layer chunks simultaneously and thus enables full layer-parallelism. Our goal is to have a training methodology scalable in the number of layers, e.g., doubling the number of layers and the number of compute resources should result in a near constant runtime. To achieve this, we leverage recent advances in parallel-in-time integration methods for unsteady differential equations [23]. Clearly, the forward propagation through a ResNet (1.2) can be seen as a discretization of a time-dependent ordinary differential equation (ODE), which was also observed in [32, 18]. Based on this interpretation, we employ a multigrid reduction in time approach [19, 20] that recursively divides the time domain – which, in this interpretation, corresponds to the layer domain – into multiple time chunks that can be processed in parallel on different compute units. Coupling of the chunks is achieved through a coarse-grid correction scheme that propagates information across chunk interfaces on a coarser time- (i.e. layer-) grid. The method can be seen as a parallelization of the model, however we employ full model-parallelism on the algorithmic level, processing layer chunks simultaneously within the iterative multigrid scheme thus breaking the traditional layer-serial propagation. At convergence, the iterative multigrid scheme solves the same problem as a layer-serial method and it can thus be integrated into any common gradient-based optimization technique to update the network parameters, such as the stochastic gradient descent (SGD) or other batch approaches. Further, it can be applied in addition to any data-parallelism across the data set elements. Runtime speedup over traditional layer-serial methods can be achieved through the new dimension of parallelization across layers enabling greater concurrency.

The addition of layer-parallelism allows for ResNets to take advantage of large machines currently programmed with message-passing style parallelism. The use of such large machines in conjunction with a multilevel training algorithm scalable in the number of layers, opens the door to training networks with thousands, or possibly even millions of layers. We demonstrate the feasibility of such an approach by using the parallel-in-time package XBraid [50] with a ResNet on large clusters. Additionally, the non-intrusive approach of XBraid would allow for any node-level optimizations (such as those utilizing GPUs) to be used.

The iterative nature of the multigrid approach further enables the use of simultaneous optimization algorithms for training the network. Simultaneous optimization methods have been widely used for PDE-constrained optimization, where they show promise for reducing the runtime overhead of the optimization when compared to a pure simulation of the underlying PDE (see e.g. [7, 51, 5] and references therein). They aim at solving the optimization problem in an all-at-once fashion, updating the optimization parameters simultaneously while solving for the time-dependent system state. Here, we apply the One-shot method [9, 31] to solve the training problem simultaneously for the network state and parameters. In this approach, network parameter updates are based on
inexact gradient information resulting from early stopping of the layer-parallel multigrid iteration.

The paper is structured as follows: Section 2 gives an introduction to the deep learning optimization problem and its interpretation as an optimal control problem. Further, it discusses numerical discretization of the optimal control problem and summarizes necessary conditions for optimality as well as commonly used numerical optimization techniques. We then introduce the layer-parallel multigrid approach replacing the forward and backward propagation through the network in Section 3. Section 4 focuses on the integration of the layer-parallel multigrid scheme into conventional as well as simultaneous optimization methods. Numerical results demonstrating the feasibility and runtime benefits of the proposed layer-parallel multigrid scheme as well as its utilization in simultaneous training are presented in Section 5.

2 Deep Learning as a Dynamic Optimal Control Problem

In this section, we present an optimal control formulation of a supervised classification problem using a deep neural network. Limiting the discussion to this specific task allows us to provide a self-contained mathematical description. We note that our techniques can be extended to other learning tasks, e.g., semi-supervised learning or auto-regression and refer to [28] for a comprehensive overview of deep learning techniques.

2.1 Optimal Control Formulation

In supervised classification, we are given some feature vectors \( y_1, y_2, \ldots, y_s \in \mathbb{R}^n \) (examples) and associated class probability vectors \( c_1, c_2, \ldots, c_s \in \Delta_n \), where \( \Delta_n \) denotes the unit simplex in \( \mathbb{R}^n \). The \( j \)-th component of \( c_k \) represents the probability of example \( y_k \) belonging to the \( j \)-th class.

The learning problem aims at training a function that approximates the feature-to-class mapping. In other words, we seek to find a function \( f(\cdot, \theta) \) and its parameter (or weights) \( \theta \) such that

\[
f(y_k, \theta) \approx c_k, \quad \text{for all } k = 1, 2, \ldots, s.
\]

In order to classify the feature vectors into specific classes, a hypothesis function is required that predicts the class probabilities of each example. Here, we limit ourselves to multinomial regression models, which are common in deep learning. To this end, we assume that the weights \( \theta \) can be partitioned into a matrix \( W \in \mathbb{R}^{n_c \times n} \) and a bias vector \( \mu \in \mathbb{R}^{n_c} \). For a generic example \( y \), the following softmax hypothesis function can then be considered:

\[
s(y, W, \mu) = \frac{1}{\mathbf{e}^{\top}_{n_c} \exp(z)} \exp(z), \quad z = Wy + \mu, \tag{2.3}
\]

where \( \mathbf{e}_{n_c} \in \mathbb{R}^{n_c} \) is a vector of all ones and \( \exp \) is the exponential function.\(^1\) It is easy to verify that \( s(y, W, \mu) \) will be in the unit simplex and can thus be seen as a discrete probability and is comparable to the corresponding class probability vector \( c \). To measure the performance of the classifier, we use the cross entropy loss function

\[
\ell(y, W, \mu, c) = -c^\top \log(s(y, W, \mu)) \tag{2.4}
\]

\[
= -c^\top z + \log(\mathbf{e}^{\top}_{n_c} \exp(z)). \tag{2.5}
\]

\(^1\)Note, that the softmax hypothesis function is invariant to scalar shifts in \( z \). Thus, without loss of generality we assume that the entries in \( z \) are non-negative, which avoids overflow.
Minimizing the average loss function over many examples with respect to $W$ and $\mu$ corresponds to finding hyperplanes that approximately partition the feature space into $n_c$ subsets. The multinomial regression model will however only be effective when the different classes can be approximately separated using hyperplanes. If this assumption is not valid, it is sometimes possible to apply nonlinear transformations to the example data that improve the performance of the above classification. The key idea in deep learning is to represent this nonlinear transformation using a neural network consisting of a concatenation of many hidden layers. Each layer transforms the input features using relatively simple operations: Each layer applies affine transformations and element-wise nonlinearities, whose parameters need to be learned along with the weights and bias of the classifying softmax function.

A powerful class of networks that has been shown to be very successful in many benchmark tasks are Residual Neural Networks (ResNets) [34]. In an abstract form, an $N$-layer residual neural network reads

$$u^{n+1} = u^n + hF(u^n, \theta^n), \quad \text{for } n = 0, 1, \ldots, N - 1, \quad \text{with } u_0 = F_{\text{in}}(y, \theta_{\text{in}}). \quad (2.6)$$

The layer transformations $F$ and $F_{\text{in}}$ consist of an affine linear transformations and element-wise nonlinearities that are parameterized by the entries in $\theta^0, \ldots, \theta^{N-1}$, and $\theta_{\text{in}}$, respectively. There are several options to model these functions. For simplicity, we consider the single layer perceptron models

$$F(u, \theta) = \sigma(K(\theta^{(1)})u + B\theta^{(2)}), \quad \text{and} \quad F_{\text{in}}(y, \theta) = \sigma(K_{\text{in}}(\theta^{(1)})y + B_{\text{in}}\theta^{(2)}), \quad (2.7)$$

where $\sigma : \mathbb{R} \rightarrow \mathbb{R}$ is a nonlinear activation function that is applied component-wise, e.g., $\sigma(x) = \tanh(x)$ or $\sigma(x) = \max\{x, 0\}$. Here, the weight vectors $\theta^n$ are partitioned into one part that defines a linear operator $K$ and another part that represents coefficients of a bias with respect to columns of the given matrices $B$ and $B_{\text{in}}$. In this work, we assume that the linear operators $K(\cdot)$ are either dense matrices or correspond to convolutional operators (see [43]) parametrized by $\theta^{(1)}$, whose entries we determine in the training. However, our method can be extended to other parameterizations (e.g., antisymmetric matrices to enforce stability [32]). While $K(\cdot)$ needs to be a square matrix we use a non-square model for the operator $K_{\text{in}}(\cdot)$ to increase the dimensionality of the dataset, which helps in the training.

Considering a small but positive $h$ in (2.6), it is intuitive to interpret ResNets as a forward Euler discretization of the initial value problem

$$\partial_t u(t) = F(u(t), \theta(t)), \quad t \in [0, T], \quad \text{with } u(0) = F_{\text{in}}(y, \theta_{\text{in}}). \quad (2.8)$$

In this formulation, $t$ is an artificial time that refers to the propagation of the input features through the neural network. The final time $T$ and the norm of $F(u(t), \theta(t))$ are loosely related to the depth of the neural network.

Replacing the original features $y$ in (2.3) by the state of (2.8) at the final time $T$, leads to the final model function

$$f(y, \theta) = s(u(T), W, \mu), \quad \text{where } u \text{ solves (2.8)}.\,$$

Minimizing the empirical cross entropy loss function leads to the continuous-in-time optimal control
\begin{equation}
\min_{u_1, \ldots, u_s, \theta, W, \mu} \frac{1}{s} \sum_{k=1}^{s} \ell(u_k(T), W, \mu, c_k) + R(\theta(t), W, \mu) \tag{2.9}
\end{equation}

subject to \begin{align*}
\partial_t u_k(t) &= F(u_k(t), \theta(t)), \quad \forall t \in [0, T], \tag{2.10} \\
u_k(0) &= F_{\text{in}}(y_k, \theta_{\text{in}}). \tag{2.11}
\end{align*}

The objective function consists of the average loss over all examples, hence approximating its expected value, and an additional regularization term denoted by \( R \) that involves all network parameters \( \theta(t) \) and the classification weights and biases \( W, \mu \). In conventional deep learning approaches, \( R \) typically applies a Tikhonov regularization that penalizes “large” network and classification parameters, measured in a chosen norm. Within the time-continuous optimal control interpretation, we additionally penalize the time derivative of \( \theta(t) \) in order to ensure weights that vary smoothly in time. This is an important ingredient for stability analysis [32]. Another task for the regularization function is to avoid over-fitting, which means that the optimal parameters perform very well for the training data but perform poorly on new data. In contrast to many applications in optimal control, in most applications of machine learning it is therefore not desirable to minimize the loss over the training data to a very high accuracy, but rather to stop the iterative minimization method early; see discussions in Sec. 2.4 and [11].

To gauge the network’s performance on unseen data it is common to set aside parts of the data as a validation set and monitor the loss over this set while adjusting hyper-parameters, e.g., the network size, layer designs, regularization parameters, optimization parameters.

\section{2.2 Discretization of the Optimal Control Problem}

We solve the continuous-in-time optimal control problem in a first-discretize-then-optimize fashion. For simplicity, we discretize the control \( \theta(t) \) and the states \( u(t) \) at regularly spaced time points \( t_n = n \cdot h \), where \( h = T/N \) and \( n = 0, 1, \ldots, N \). This leads to the discrete control problem

\begin{equation}
\min_{u_0^0, \ldots, u_s^0, \ldots, u_s^N, W, \mu, \theta} J(u_1^N, \ldots, u_s^N, W, \mu, \theta) \tag{2.12}
\end{equation}

subject to \begin{align*}
u_{k,n+1} &= \Phi(u_{k,n}, \theta), \quad \forall n = 0, \ldots, N - 1 \tag{2.13} \\
u_0^0 &= F_{\text{in}}(y_k, \theta_{\text{in}}). \tag{2.14}
\end{align*}

where \( \theta \) collects all network control parameters that need to be learned, \( \theta := (\theta^0, \ldots, \theta^{N-1}, \theta_{\text{in}}) \) and \( J \) denotes the discretized objective function

\begin{equation}
J(u_1^N, \ldots, u_s^N, W, \mu, \theta) := \frac{1}{s} \sum_{k=1}^{s} \ell(u_k^N, W, \mu, c_k) + R(\theta, W, \mu) \tag{2.15}
\end{equation}

In this general description, \( \Phi \) can denote any layer-to-layer propagator which maps data \( u^n \) to the next layer. In case of a forward Euler discretization, it reads

\begin{equation}
\Phi(u, \theta) = u + hF(u, \theta). \tag{2.16}
\end{equation}

giving the ResNet propagation as in (2.6). However, the time-continuous interpretation of the network propagation permits to employ other, possibly more stable, discretization schemes, see.
[32] and thus opens the door for new architecture designs. It also allows for discretization of the controls, $\theta$, and states, $u$, at different time points, which can improve the efficiency and is the subject of further research. Further, numerical advances for solving the corresponding optimal control can be leveraged, such as the time-parallel approach which is discussed in this paper.

### 2.3 Necessary Optimality Conditions

The necessary conditions for optimality of the discrete, equality-constrained optimization problem (2.12)-(2.14) can be derived from the associated Lagrangian function

$$
L := J(u^N_1, \ldots, u^N_s, W, \mu, \theta) + \sum_{k=1}^{s} \left[ \sum_{n=0}^{N-1} (u^{n+1}_k)^T (\Phi(u^n_k, \theta^n) - u^{n+1}_k) + (u^0_k)^T (F_{in}(y_k, \theta_{in}) - u^0_k) \right]
$$

where $\bar{u}^n_k$ denote the so-called adjoint states for layer $n = 0, \ldots, N$ and example $k = 1, \ldots, s$. Optimal points of the problem are saddle points of the Lagrangian function (see e.g. [45]), thus equating its partial derivatives with respect to $u_0, \ldots, u^N, \bar{u}^0, \ldots, \bar{u}^N, \theta_0, \ldots, \theta^N, \theta_{in}, W, \mu$ to zero yields the following necessary conditions for optimality:

1. **State equations**

$$
u^{n+1}_k = \Phi(u^n_k, \theta^n), \quad \forall n = 0, \ldots, N - 1,
$$

with $u^0_k = F_{in}(y_k, \theta_{in})$, for all $k = 1, \ldots, s$ \hfill (2.18)

2. **Adjoint equations**

$$
\bar{u}^n_k = (\partial_u \Phi(u^n_k, \theta^n))^T \bar{u}^{n+1}_k, \quad \forall n = 0, \ldots, N - 1,
$$

with $\bar{u}^N_k = \frac{1}{s} (\partial_u \ell(u^N_k, W, \mu, c_k))^T$ for all $k = 1, \ldots, s$ \hfill (2.21)

3. **Design equations**

$$
0 = \sum_{k=1}^{s} (\partial_{\theta^n} \Phi(u^n_k, \theta^n))^T \bar{u}^{n+1}_k + (\partial_{\theta^n} R(\theta, W, \mu))^T \quad \forall n = 0, \ldots, N - 1
$$

$$
0 = \sum_{k=1}^{s} (\partial_{\theta_{in}} F_{in}(y_k, \theta_{in}))^T \bar{u}^0_k + (\partial_{\theta_{in}} R(\theta, W, \mu))^T
$$

$$
0 = \frac{1}{s} \sum_{k=1}^{s} (\partial_{W} \ell(u^N_k, \mu, c_k))^T + (\partial_{W} R(\theta, W, \mu))^T
$$

$$
0 = \frac{1}{s} \sum_{k=1}^{s} (\partial_{\mu} \ell(u^N_k, W, \mu, c_k))^T + (\partial_{\mu} R(\theta, W, \mu))^T
$$

Here, subscripts denote partial derivatives, $\partial_x = \frac{\partial}{\partial x}$. The state equations correspond to the forward propagation of input data $y_k$ through the network layers. The adjoint equations propagate partial derivatives with respect to the network states backwards through the network layers, starting
from a terminal condition at $N$ equal to the local derivative of the loss function. In a time-
continuous setting, the adjoint equations correspond to the discretization of an additional adjoint
dynamical system for propagating network state derivatives backwards in time.\footnote{The adjoint approach is a common and well-established method in optimal control that provides gradient information at computational costs that are independent of the design space dimension, see e.g. \cite{26}} We note that
solving the above adjoint equations backwards in time is equivalent to the backpropagation
method that is established within the deep learning community for computing the network gradient \cite{43}. It further corresponds to the reverse mode of automatic differentiation \cite{29}. The adjoint variables
are utilized in the right-hand-side of the design equations, which then form the so-called reduced
gradient. For feasible state and adjoint variables, the reduced gradient holds the total derivative,
i.e. the sensitivity, of the objective function with respect to the controls. It is thus used within
gradient-based optimization methods for updating the network controls.

Training a residual network corresponds to the attempt of solving the above set of equations
for the special choice of $\Phi$ being the forward Euler time-integration scheme. However, the above
equations, as well as the discussions in the remainder of this paper, are general, in the sense that
any other layer-to-layer propagator $\Phi$ can be utilized that corresponds to the discretization of the
dynamical system (2.8).

\textbf{Remark 1} The adjoint equations depend on the primal states $u_k^\Phi$ themselves. Therefore, those
states need to be either stored during forward propagation, or recomputed while solving the adjoint
equations. Hybrid approaches like the check-pointing method have been developed within the op-
timal control and unsteady PDE-constrained optimization community, which compromise memory
consumption with computational complexity (see, e.g., \cite{49}). Memory-free methods using reversible
networks were first proposed for general dynamics in \cite{27}. However, as shown in \cite{14}, not all
architectures that are reversible algebraically are forward and backward stable numerically. This
motivates limiting the forward propagation to stable dynamics, e.g., inspired by hyperbolic systems.

\subsection{2.4 Common Gradient-based Training Techniques}

Due to the large-scale and stochastic nature of the learning problem (2.12), it is common to
use stochastic approximation schemes, such as variants of the stochastic gradient descent (SGD)
method, for updating the controls within a gradient-based optimization iteration. These methods
assemble gradient information from a (randomly chosen) subset of the training data, i.e. the sum
over $k$ in the design equations cover only a subset $k \in S \subseteq \{1, \ldots, s\}$ of the full data, called a \textit{batch}.
The size of the batch can be as small as one, where a different example is randomly chosen in each
iteration of the SGD method. While they reduce the cost of gradient evaluations, small batch sizes
complicate their data-parallel implementation when more computational resources than examples
in the batch are available. An alternative are stochastic average approximation (SAA) schemes
that allow for larger batch sizes and the straightforward incorporation of second-order information,
such as standard (quasi-) Newton type methods (e.g. L-BFGS, etc.). See, e.g., \cite{11} for an overview
and comparison of past and current optimization techniques in machine learning.

In all of the above approaches, each iteration of the (sub-) gradient-based optimization approach
requires a forward propagation of (a batch of) data through every layer, followed by the loss
evaluation and a backpropagation again through every layer in order to evaluate the gradient.
The sequential nature of these layer propagations create a major bottleneck for fast and scalable
training since runtimes increase linearly with the number of layers. The next section explains
3 Layer-Parallel Multigrid Approach

In order to achieve concurrency across all the network layers, we replace the serial layer propagation through the residual network with an iterative multigrid scheme. This iterative multigrid scheme solves the same equations, that standard serial propagation solves directly. The key difference is that the iterative multigrid scheme allows all layers to be processed concurrently, and in parallel.

Based on the time-continuous nonlinear dynamics interpretation of ResNets as in (2.8), and its time-discretization as in (2.13), we employ the multigrid reduction in time (MGRIT) [19] method to parallelize across the time domain of the network. While the discussion in this section revolves around time-grids, here each time point is considered a layer in the network. Thus, the multigrid approach constructs a multilevel hierarchy, where each level is a network containing fewer layers (i.e., fewer time points). The coarsest level will contain only a handful of layers, while the finest level could contain thousands (or more) of layers. When run in parallel, each compute unit will own only a few layers, thus allowing for massive parallelism to be applied to the learning algorithm.

The MGRIT scheme was first introduced in [19] and first applied to neural networks in [47], although that work considered parallelism over epochs of the training algorithm, not layers. We refer to the works [19, 20, 30] for the details of the method, but we will here provide a self-contained overview of the MGRIT scheme.

3.1 Multigrid-in-Layer for Forward Propagation

The MGRIT algorithm solves the forward problem (2.18)–(2.19). Collecting all network states into a vector \(U = (u^0, u^1, \ldots, u^N)\), this forward problem can be written as the space-time system

\[
A(U, \theta) := \begin{pmatrix}
  I & -I & I & \cdots & I \\
  -I & I & -I & \cdots & -I \\
  \vdots & \ddots & \ddots & \ddots & \vdots \\
  -I & \cdots & -I & I & -I \\
  I & -I & \cdots & -I & I
\end{pmatrix}
\begin{pmatrix}
u^0 \\
u^1 \\
\vdots \\
u^N
\end{pmatrix} - h
\begin{pmatrix}
  F(u^0, \theta^0) \\
  F(u^1, \theta^1) \\
  \vdots \\
  F(u^{N-1}, \theta^{N-1})
\end{pmatrix} =
\begin{pmatrix}
  F_{\text{in}}(y, \theta_{\text{in}}) \\
  0 \\
  \vdots \\
  0
\end{pmatrix} = G. \tag{3.26}
\]

For a forward Euler discretization of the layer-to-layer propagator \(\Phi\) (i.e. a ResNet architecture, see (2.16)), it reads

\[
A(U, \theta) = \begin{pmatrix}
  I & -I & I & \cdots & I \\
  -I & I & -I & \cdots & -I \\
  \vdots & \ddots & \ddots & \ddots & \vdots \\
  -I & \cdots & -I & I & -I \\
  I & -I & \cdots & -I & I
\end{pmatrix}
\begin{pmatrix}
u^0 \\
u^1 \\
\vdots \\
u^N
\end{pmatrix} - h
\begin{pmatrix}
  0 \\
  F(u^0, \theta^0) \\
  F(u^1, \theta^1) \\
  \vdots \\
  F(u^{N-1}, \theta^{N-1})
\end{pmatrix} =
\begin{pmatrix}
  F_{\text{in}}(y, \theta_{\text{in}}) \\
  0 \\
  \vdots \\
  0
\end{pmatrix} = G. \tag{3.27}
\]

Here, the \(u^n\) denote the time steps of the forward problem for either a single generic input vector \(y\) or for a batch, i.e. a subset, of input vectors \(y_k, k \in S \subset \{1, \ldots, s\}\). Sequential time stepping solves (3.26) through forward substitution, i.e. forward propagation of input data through the network layers. On the other hand, MGRIT solves (3.26) iteratively, beginning with some initial
solution guess for $U$, by using the Full Approximation Storage (FAS) nonlinear multigrid method [12], see Section 3.1.1. In both cases, the exact same equations are solved and thus the same solution is reached (in the case of MGRIT, to within a user tolerance). Regarding cost, sequential time-stepping is $O(N)$, but sequential. Instead, MGRIT solves this system with an $O(N)$ multigrid method with a larger computational constant, but with parallelism in the layer dimension. This parallelism allows for a distributed workload, processing multiple layers in parallel on multiple compute units. Typically, a certain number of processors are needed for MGRIT to show a speedup over layer-serial forward propagation. This is referred to as the cross-over point. However, the speedups observed can be large, e.g., the work [31] showed a speedup of 19x for a model optimization problem while using an additional 256 processors in time.

In summary, each block row in equation (3.26) corresponds to a time-step, which in turn corresponds to a layer in the network. Thus, the parallelism provided by MGRIT is over all time-steps, and this translates to a parallelism over all layers. Additionally, MGRIT can be applied within any training algorithm that can be formulated as a dynamic optimal control problem, as in Section 2. This includes common algorithms like stochastic gradient descent, where MGRIT would solve system(s) of the form (3.26), but where the respective feature vectors $y$ are selected from a random distribution.

3.1.1 MGRIT using Full Approximation Scheme (FAS)

Similar to linear multigrid methods, the nonlinear FAS method computes coarse-grid error corrections to fine-grid approximations of the solution.\(^3\)

Each iteration of the nonlinear MGRIT scheme consists of three steps: First, a relaxation scheme is used to cheaply compute an approximation to the true solution on the fine-grid. Then, the error is approximated on a coarser grid by solving a coarse-grid residual equation. Lastly, the interpolated coarse-grid error approximation is used to correct the current fine-grid solution approximation. This idea is based on the fact that low frequency error components can be smoothed out much faster on coarser grids. While a general introduction to linear and nonlinear multigrid methods can be found in [13], we explain here each of the algorithmic components as realized in MGRIT, starting with the coarse-grid residual equation.

Let $U$ denote an approximation to the true solution $U^*$ of (3.26) such that $U^* = U + E$ with

---

\(^3\)For further motivation, the linear case may be considered. Here, sequential time-stepping is equivalent to forward substitution with a block lower bidiagonal system. MGRIT replaces this sequential forward solve with an iterative solve using multigrid reduction, which is strongly related to approximate block cyclic reduction methods. See [19].

---
\( \mathbf{E} \) denoting the current error. Then this error can be expressed in terms of the residual \( \mathbf{R} \) as

\[
\mathbf{R} := \mathbf{G} - \mathbf{A}(\mathbf{U}, \mathbf{\theta}) = \mathbf{A}(\mathbf{U}, \mathbf{\theta}) - \mathbf{A}(\mathbf{U}, \mathbf{\theta}) = \mathbf{A}(\mathbf{U} + \mathbf{E}, \mathbf{\theta}) - \mathbf{A}(\mathbf{U}, \mathbf{\theta}).
\]

(3.28)

In a multigrid setting, this residual equation (3.29) is solved on a coarser grid such that an approximation to the error \( \mathbf{E} \) can be computed more cheaply than on the fine-grid. In linear cases, i.e. when \( \mathbf{A} \) is linear in \( \mathbf{U} \), the residual equation reduces to \( \mathbf{A}\mathbf{E} = \mathbf{R} \) and can thus be solved for the error \( \mathbf{E} \) directly. However, in the nonlinear case, the equation \( \mathbf{A}(\mathbf{V}, \mathbf{\theta}) = \mathbf{A}(\mathbf{U}, \mathbf{\theta}) + \mathbf{R} \) is solved for \( \mathbf{V} \) on the coarse grid before the error can be extracted with \( \mathbf{E} = \mathbf{V} - \mathbf{U} \).

For a given time-grid discretization \( t_n = nh, n = 0, \ldots, N \) and \( h = T/N \), the coarse grid is defined by choosing a coarsening factor \( c > 1 \) and assigning every \( c \)-th time point to the next coarser time-grid with \( T_n = nh, n = 0, \ldots, N \), and the coarse-grid spacing \( h = ch \). An example of two grid levels using a coarsening factor of \( c = 5 \) is given in Figure 1. The residual \( \mathbf{R} \) as well as the current approximation \( \mathbf{U} \) and controls \( \mathbf{\theta} \) are restricted to the coarse grid with injection by choosing every \( c \)-th time-point, i.e., the restriction of \( \mathbf{U} \) is

\[
\mathbf{U}_\Delta = (\mathbf{u}_\Delta^0, \mathbf{u}_\Delta^1, \ldots, \mathbf{u}_\Delta^N), \text{ where } \mathbf{u}_\Delta^i = \mathbf{u}_c^i,
\]

(3.30)

with \( \mathbf{R}_\Delta, \mathbf{\theta}_\Delta \) defined analogously. Consequently, the coarse-grid residual equation that is to be solved reads

\[
\mathbf{A}_\Delta(\mathbf{V}_\Delta, \mathbf{\theta}_\Delta) = \mathbf{A}_\Delta(\mathbf{U}_\Delta, \mathbf{\theta}_\Delta) + \mathbf{R}_\Delta.
\]

(3.31)

Here, \( \mathbf{A}_\Delta \) denotes a re-discretization of \( \mathbf{A} \) on the coarse grid utilizing a coarse-grid propagator \( \Phi_\Delta \), i.e.,

\[
\mathbf{A}_\Delta(\mathbf{U}_\Delta, \mathbf{\theta}_\Delta) := \begin{pmatrix}
\mathbf{u}_\Delta^0 \\
\mathbf{u}_\Delta^1 - \Phi_\Delta(\mathbf{u}_\Delta^0, \mathbf{\theta}_\Delta^0) \\
\vdots \\
\mathbf{u}_\Delta^N - \Phi_\Delta(\mathbf{u}_\Delta^{N\Delta-1}, \mathbf{\theta}_\Delta^{N\Delta-1})
\end{pmatrix}
\]

(3.32)

An obvious choice for \( \Phi_\Delta \) is a re-discretization of the problem on the coarse grid, such as by using the same propagator as on the fine grid, but with a bigger time step \( h = ch \), thus skipping the fine-grid time points and updating only the coarse-grid points. For instance, \( \Phi \) could be a forward or backward Euler discretization with time-step size \( h \), and \( \Phi_\Delta \) could be a forward or backward Euler discretization with time-step size \( h = ch \). In the case of forward Euler (i.e., ResNet architecture), the coarse-grid propagator \( \Phi_\Delta \) is given by

\[
\Phi_\Delta(\mathbf{u}_\Delta^0, \mathbf{\theta}_\Delta^0) = \mathbf{u}_\Delta^0 + h_\Delta F(\mathbf{u}_\Delta^0, \mathbf{\theta}_\Delta^0).
\]

(3.33)

On the coarse grid, the residual equation (3.31) is solved exactly with forward substitution. Afterwards, the error approximation on the coarse grid is extracted with \( \mathbf{E}_\Delta = \mathbf{V}_\Delta - \mathbf{U}_\Delta \). This coarse-grid error approximation is then used to correct the fine-grid approximation \( \mathbf{U} \) at coarse-grid points with \( \mathbf{U}_c := \mathbf{U}_c + \mathbf{E}_\Delta \).

Complementing the coarse time-grid error correction is the relaxation process on the fine time-grid, which in addition to the coarse-grid correction also provides an improved approximation to
Figure 2: F-relaxation and C-relaxation for a coarsening by factor of $c = 5$.

$\Phi$ $\Phi$ $\Phi$ $\Phi$ $\Phi$ $\Phi$ $\Phi$ $\Phi$ $\Phi$ $\Phi$ $\Phi$

F-relaxation

$\Phi$ $\Phi$

C-relaxation

U. Here, block Jacobi relaxation alternates between the fine-points and the coarse-points (black, vertical line F-points and red circle C-points in Figure 1). More precisely, relaxation on the fine-points (called F-relaxation) corresponds to updating each fine-point concurrently over each interval of fine-points, thus propagating each coarse-point value $u^{kc}$ through the corresponding fine-point interval $(T^k, T^{k+1})$ as in

$$ u^n \leftarrow \Phi(u^{n-1}, \theta^{n-1}), \quad \text{for each } n = kc + 1, kc + 2, \ldots, (k + 1)c - 1. \quad (3.34) $$

Importantly, each $k$-th interval of F-points can be computed independently, in parallel. Relaxation on the coarse-points (called C-relaxation) is analogous, and updates each coarse-point concurrently by propagating the nearest left neighboring value. For the $k$-th coarse-point, the update is given by

$$ u^{kc} \leftarrow \Phi(u^{kc-1}, \theta^{kc-1}), \quad \text{for } k = 1, 2, \ldots, N_\Delta. \quad (3.35) $$

The actions of F- and C- relaxation is depicted in Figure 2. Unless otherwise noted, we use FCF-relaxation, which is an application of F-relaxation (3.34), followed an application of C-relaxation (3.35), and then F-relaxation (3.34) again. We note that such F/C orderings in relaxation is common for multigrid methods.

Taken together, the coarse-grid error correction and the fine-grid relaxation form the two-grid MGRIT cycle depicted in Algorithm 1. Typically, the MGRIT Algorithm 1 is carried out recursively, with successively coarser time-grids, until a coarsest time-grid of trivial size is reached, and Step 3 is solved exactly using forward substitution. If the levels are traversed in order, going down to the coarsest time-grid and then back to the finest time-grid, this is called a V-cycle. It corresponds to the “Solve” in Step 3 being implemented as a single recursive call. However, more powerful cycles that visit coarse time-grids more frequently are available, e.g., F-cycles. See Figure 3 for cycling examples, and [48, 13] for more information on multigrid cycling.

Note that the main work carried out on a given time-grid is the parallel relaxation process. Thus the work on each MGRIT level is highly parallel. Only when a coarsest time-grid of trivial size is reached, the level is solved sequentially by forward substitution. Thus, the algorithm simultaneously computes all time-steps in parallel, reducing the serial propagation component to the size of the coarsest grid plus the traversal through each level.

Before starting MGRIT, an initial solution guess for $U$ must be set. Typically, the coarse-grid points are initialized using the best current solution estimate. This is often either some generic initial condition, or an interpolated solution from a cheaper coarser time-grid.

$\Phi$ $\Phi$

The F-relaxation two-grid version of nonlinear MGRIT is equivalent to the Parareal algorithm [24].
Algorithm 1 MGRIT($A, U, \theta, G$) for two grid levels

1: Apply F- or FCF-relaxation to $A(U, \theta) = G$ \hspace{1cm} $\triangleright$ eq. (3.34)–(3.35)
2: Restrict the fine grid approximation and residual $R$ to the coarse grid:
   $U^i_\Delta \leftarrow U^{ic}, R^i_\Delta \leftarrow (G - A(U, \theta))^{ic}$, for $i = 0, \ldots, N_\Delta$
3: Solve $A_\Delta(V_\Delta, \theta_\Delta) = A_\Delta(U_\Delta, \theta_\Delta) + R_\Delta$. \hspace{1cm} $\triangleright$ eq. (3.31)
4: Compute the coarse-grid error approximation: $E_\Delta = V_\Delta - U_\Delta$.
5: Correct $U$:
   $U^{ic} \leftarrow U^{ic} + E^{ic}$, for $i = 0, \ldots, N_\Delta$, and apply F-relaxation
6: If $\|R\| \leq \text{tol}$: halt.
   Else: go to step 1.

Figure 3: Depiction of one V-cycle and one F-cycle with four levels. Level $\ell = 0$ is the fine
time-grid. The arrows denote the order that the grids are traversed.

3.1.2 Fix-point formulation

Mathematically, the MGRIT algorithm can be considered a fixed-point method for solving the
forward problem (2.18)–(2.19). Using the iteration index $m$, it reads

$$U_{m+1} = \text{MGRIT}(A, U_m, \theta, G),$$ \hspace{1cm} (3.36)

The MGRIT iterator has been shown to be a contraction in many settings for linear, nonlinear,
parabolic, and hyperbolic problems, although hyperbolic problems tend to be more difficult (e.g.,
[17, 19, 31, 21]). Upon convergence, the limit fixed-point $U = \text{MGRIT}(A, U, \theta, G)$ will satisfy
the discrete network state equations as in (2.13)–(2.14), since MGRIT solves the same underlying
problem.

3.2 Multigrid-in-Layer for Backpropagation

While section 3.1 introduces the layer-parallel MGRIT approach for replacing the forward propa-
gation, similarly the same scheme can be utilized for solving the adjoint equations (2.20) – (2.21)
and thus replacing the layer-serial backpropagation. The adjoint equations run backwards through
the layers and are linear in $\bar{u}^n$, thus the adjoint system that is to be solved with MGRIT reads

$$\begin{bmatrix}
   I \\
   -(\partial_u \Phi^0)^T & I \\
   -(\partial_u \Phi^1)^T & I \\
    \vdots & \vdots \\
   -(\partial_u \Phi^{N-1})^T & I
\end{bmatrix}
\begin{bmatrix}
   \bar{u}_N \\
   \bar{u}_{N-1} \\
    \vdots \\
   \bar{u}^1 \\
   \bar{u}^0
\end{bmatrix}
= \begin{bmatrix}
   \frac{1}{s}(\partial_u \bar{u}^N \ell^N)^T \\
   0 \\
    \vdots \\
   0
\end{bmatrix},$$ \hspace{1cm} (3.37)
where again \( \bar{u}^n \) denotes the adjoint variable at layer \( n \) for a general example \( y \) or for a batch of examples \( y_k, k \in S \subset \{1, \ldots, s\} \). Further, \( (\partial_u \Phi^n)^T \) denotes the partial derivative \( \partial_u \Phi(u^n, \theta^n)^T \). It corresponds to the backwards layer-propagation of adjoint sensitivities which in the case of a forward Euler discretization for \( \Phi \) (i.e., ResNet architecture), reads

\[
\partial_u \Phi(u^n, \theta^n)^T \bar{u}^{n+1} = \bar{u}^{n+1} + h \partial_u F(u^n, \theta^n)^T \bar{u}^{n+1}. \quad (3.38)
\]

Each backward propagator at layer \( n \) depends on the primal state \( u^n \), hence the system matrix and right-hand-side of (3.37) depend on the current state \( U \) which is reflected in the subscript \( A_U \) and \( G_U \). The structure of the adjoint system (3.37), however, is the same as that of the state system (3.27). Hence the same MGRIT approach as presented in Algorithm 1 can be utilized to solve the adjoint equations with the layer-parallel multigrid scheme by applying the following iteration

\[
\bar{U}_{m+1} = \text{MGRIT}(A_U, \bar{U}_m, \theta, G_U); \quad (3.39)
\]

for the adjoint vector \( \bar{U} := (\bar{u}^N, \ldots, \bar{u}^0) \).

### 3.3 Non-intrusive implementation

The MGRIT algorithm relies on the action of the layer-to-layer forward and backward propagators, \( \Phi \) and \( \partial_u \Phi^T \), and their respective re-discretizations, \( \Phi_\Delta \) and \( \partial_u \Phi_\Delta^T \), on coarser grid levels. However, it does not access or “know” the internals of these functions. Hence, MGRIT can be applied in a fully non-intrusive way with respect to any existing discretization of the nonlinear dynamics describing the network forward and backward propagation. A user can wrap existing sequential evolution operators according to an MGRIT software interface, and then the MGRIT code iteratively computes the solution to (2.18)–(2.19) and (2.20)–(2.21) in parallel.

Our chosen MGRIT implementation for time-parallel computations (forwards and backwards) is XBraid [50]. One particular advantage of XBraid is its generic and flexible user-interface that requires relatively straight-forward user-routines which likely already exist, such as how to take inner-products and norms with vectors \( u^n \), how to take a time-step with \( \Phi \) and \( \partial_u \Phi^T \), etc. For more details on the various user-defined functions, see the simple examples included with the package [50].

Since the user defines the action of \( \Phi \), any existing implementation of layer computations can continue to be used, including accelerator code, e.g., for GPUs. The internals of \( \Phi \) are completely opaque to XBraid. However since \( \Phi \) takes a single time-step, any use of GPU kernels for \( \Phi \) implies memory movement to and from the CPU every time-step. This is because current architectures largely rely on the CPU to handle the message passing layer of parallelism, and it is over this layer that XBraid provides temporal parallelism. However, future implementations could move the message passing layer to occur solely on the GPU, thus removing this memory movement overhead. Additionally, the bandwidth and latency between CPUs and accelerators will continue to improve, also ameliorating this issue.

In [31], the XBraid library was extended with the ability to compute parallel-in-time gradients based on automatic differentiation (AD). The AD-based adjoint iteration solves the state and adjoint equations simultaneously with MGRIT such that gradients of the objective function are computed alongside the state computation.
4 Simultaneous Layer-Parallel Training

The state and adjoint MGRIT iterations described in Section 3 recover at convergence the same reduced gradient as a serial forward- and backpropagation through the network. They can thus be integrated into any gradient-based training algorithm for updating the network control parameters $\theta, W, \mu$. Sub-gradient methods, such as SGD or other batch approaches can also be utilized by choosing the subset $S \subset \{1, \ldots, s\}$ correspondingly. The layer-parallel computations are particularly attractive in the small-batch mode when options for data parallelism are limited. Thus, we expect a runtime speedup over a layer-serial approach for deep networks through the greater concurrency within the state and adjoint solves, when the computational resources are large enough.

In order to speed up the training process even further, this section introduces a simultaneous training algorithm that solves the network state and adjoint inexactly during training and thus performs network parameter updates based on inexact gradient information. We thus aim at solving the necessary optimality conditions of the training problem in an all-at-once fashion, where state, adjoint and design equations are updated in a coupled iteration simultaneously.

To this end, we reduce the accuracy of the state and adjoint MGRIT solver during training and update the network control parameters utilizing inexact gradient information. This corresponds to an early stopping of the MGRIT iterations in each outer optimization cycle. The idea and theoretical background of this early-stopping approach of the inner fixed-point iteration for the state and adjoint equations is based on the One-shot method [9], which has proven successful in reducing the computational costs for PDE-constrained optimization, mostly in aerodynamic applications [38, 25, 8]. Here, it has been observed that the cost for a simultaneous One-shot optimization is only a small multiple of the cost of a pure simulation of the underlying fixed-point algorithm [3]. Here, we expect a runtime speedup over a layer-serial approach for deep networks through the greater concurrency within the state and adjoint solves, when the computational resources are large enough.

Algorithm 2 Simultaneous One-shot optimization

1: Perform $m_1$ state updates $\triangleright$ layer-parallel on $p$ processors
   for $m = 1, \ldots, m_1$ : $U_m \leftarrow \text{MGRIT}(A, U_{m-1}, \theta, G)$
2: Perform $m_2$ adjoint updates $\triangleright$ layer-parallel on $p$ processors
   for $m = 1, \ldots, m_2$ : $\bar{U}_m \leftarrow \text{MGRIT}(A U_{m_1}, \bar{U}_{m-1}, \theta, G U_{m_1})$
3: Assemble gradient
   \[
   \nabla_{\theta}^n J = \sum_{k \in S} \left( \partial_{\theta^n} \Phi(u_{k,m_1}^n, \theta^n) \right)^T \bar{u}_{k,m_2}^{n+1} + \left( \partial_{\theta^n} R(\theta, W, \mu) \right)^T, \quad \forall n = 0, \ldots, N-1
   \]
   \[
   \nabla_{\theta}^n J = \sum_{k \in S} \left( \partial_{\theta^n} F_{in}(y_k, \theta_{in}) \right)^T u_{k,m_2}^0 + \left( \partial_{\theta^n} R(\theta, W, \mu) \right)^T
   \]
   \[
   \nabla_{W} J = \frac{1}{|S|} \sum_{k \in S} \left( \partial_{W} \ell(u_{k,m_1}^N, W, \mu, c_k) \right)^T + \left( \partial_{W} R(\theta, W, \mu) \right)^T
   \]
   \[
   \nabla_{\mu} J = \frac{1}{|S|} \sum_{k \in S} \left( \partial_{\mu} \ell(u_{k,m_1}^N, W, \mu, c_k) \right)^T + \left( \partial_{\mu} R(\theta, W, \mu) \right)^T
   \]
4: Approximate the Hessians $B_{\theta}, B_{W}, B_{\mu}$ and select a stepsize $\alpha > 0$
5: Network control parameter update:
   $\theta \leftarrow \theta - \alpha B_{\theta}^{-1} \nabla_{\theta} J$
   $W \leftarrow W - \alpha B_{W}^{-1} \nabla_{W} J$
   $\mu \leftarrow \mu - \alpha B_{\mu}^{-1} \nabla_{\mu} J$
6: If converged: halt
   Else: go to step 1.
Algorithm 2 presents the proposed simultaneous layer-parallel One-shot training approach. To clarify the details of the algorithm, the following points need to be considered:

- **Number of state and adjoint updates $m_1, m_2$:** The numbers $m_1, m_2 \in \mathbb{N}$ determine the number of layer-parallel multigrid updates for the state and the adjoint variables in each optimization cycle. If $m_1, m_2$ are large, the solutions to the state and adjoint equations are approximated with high accuracy in each training iteration. Hence, a conventional reduced-space training approach is recovered where only the serial forward and backward propagation through the network are replaced by layer-parallel MGRIT iterations. In contrast, considering smaller numbers of inner MGRIT iterations, e.g. $m_1, m_2 \in \{1, 2\}$, yields a simultaneous optimization approach where the network state, adjoint and control variables are updated simultaneously in a coupled iteration. Hence, control updates in Step 5 are based on inexact gradient information utilizing the most recent state and adjoint variables $(\mathbf{u}_{m_1}^n, \mathbf{u}_{m_2}^n)$.

For the extreme case $m_1 = m_2 = 1$, the resulting optimization iteration can mathematically be interpreted as an approximate, reduced sequential quadratic programming (rSQP) method with convergence analysis presented in [38]. In [10], theoretical considerations on the choice of $m_1, m_2$ is presented, which rely on the accuracy of the state and adjoint residual by searching for descent on an augmented Lagrangian function. In practice, choosing $m_1, m_2$ to be as small as 2 has proven successful in our experience.

- **Hessian approximation:** In order to prove convergence of the One-shot method on a theoretical level, the preconditioners $\mathbf{B}_\theta, \mathbf{B}_W, \mathbf{B}_\mu$ should approximate the Hessian of an augmented Lagrangian function that involves the residual of the state and adjoint equations (elaborate theoretical analysis can be found in [9] and references therein). Numerically, we approximate the Hessian through consecutive limited-memory BFGS updates based on the current reduced gradient (thus assuming that the residual term is small). Alternatively, one might try to approximate the Hessian with a scaled identity matrix, which drastically reduces computational complexity and has already proven successful in various applications of the One-shot method for aerodynamic optimization. It should be noted, that the Hessian with respect to $W, \mu$ can be computed directly as it involves only the second derivative of the loss function $\ell$ in (2.5).

- **Stepsize selection:** The stepsize $\alpha$ is selected through a standard line-search procedure based on the current value of the objective function, e.g. a backtracking line-search satisfying the (strong) Wolfe-condition (see, e.g., [45]).

- **Stopping criterion:** In Step 6 of the One-shot algorithm, a criterion for convergence and hence termination needs to be chosen. Standard optimization techniques utilize a tolerance on the norm of the gradient. In contrast, since the One-shot method targets optimality and feasibility of the state and adjoint variables simultaneously, the stopping criterion should also involve the norm of the state and adjoint residuals. In the context of network training, however, solving the optimization problem to high accuracy is often not desirable in order to prevent training the network to match the specific input data set $\mathcal{Y} \times \mathcal{C}$, i.e. overfitting. The training goal is rather to find network control parameters that generalize well on data that has not been used for training, i.e. on a validation data set. A validation accuracy is therefore computed in each iteration of the above algorithm by applying the current network controls to a separate validation dataset. We terminate the optimization algorithm, if the
current network controls produce a high validation accuracy, rather than focusing on the current residuals of the state, adjoint and gradient norms.

The simultaneous layer-parallel training algorithm aims at reducing the runtime of conventional training algorithms in two ways: First, it enables a new dimension for parallelism across the network layers using the nonlinear multigrid approach, which goes in addition to data-parallelism across data elements. This allows for leveraging high-performance compute clusters to speed up the training process. Second, due to the iterative nature of the layer-parallel multigrid computation, early stopping can be applied to the state and gradient computation. Thus inexact gradient information can be utilized already while solving for the network state, targeting feasibility and optimality simultaneously.

5 Numerical Results

In this section, we investigate the computational benefits of the simultaneous layer-parallel training approach on three test cases. For each test case, we first investigate runtime scaling results of the layer-parallel MGRIT propagation for one single objective function and gradient evaluation, and compare it to conventional serial-in-layer forward- and backpropagation (Section 5.2). Then, we integrate the layer-parallel MGRIT iterations into the simultaneous training framework in Section 5.3.

For all test cases, our focus is on the ability to achieve fast training for very deep neural networks by introducing parallelism between the layers. It is likely, though not explored here, that greater combined speedups could be obtained by additionally using data-parallelism or parallelizing inside of each layer. Further studies are required to better understand the trade-off of distributing parallel work between layer-parallel and data-parallel.

5.1 Test cases

1. Level set classification (Peaks example):

As a first step, we consider the test problem suggested in [32] which consists of classifying grid points into five level sets of the smooth nonlinear function

\[ f(y_1, y_2) = 3(1 - y_1)^2 \exp(-y_1^2 - (y_2 + 1)^2) - 10(y_1/5 - x_1^3 - y_2^5) \exp(-y_1^2 - y_2^2) - 1/3 \exp(-(y_1 + 1)^2 - y_2^2). \]

The training data set consists of \( s = 5000 \) randomly chosen points \( y_k \in [-3, 3]^2, k = 1, \ldots, s \), and unit vectors \( c_k \in \mathbb{R}^5 \) which represent the probability that a point \( y_k \) belongs to level set \( i \in \{1, 2, 3, 4, 5\} \), see Figure 4. The goal is to train a network such that it predicts the correct level sets for new points in \([-3, 3]^2\) (validation points).

We choose a ResNet architecture with ReLU activation (i.e. \( \sigma(x) = \max\{0, x\} \), smoothed around zero) and define the linear operations \( K(\cdot) \) at each layer to be a dense matrix representation of the weights \( \theta^a \). We choose a network depth of \( T = 5 \) discretized with up to \( N = 2048 \) layers and a network width of 8 such that \( u^n \in \mathbb{R}^8, \forall n = 0, \ldots, N \).

2. Hyperspectral image segmentation (Indian Pines):
In this test case, we consider a soil segmentation problem based on a hyperspectral image data set. The input data consists of hypersectral bands over a single landscape in Indiana, US, (Indian Pines data set [3]) for $145 \times 145$ pixels. For each pixel, the data set contains 220 spectral reflectance bands which represent different portions of the electromagnetic spectrum in the wavelength range $0.4 - 2.5 \cdot 10^{-6}$. The goal is to classify each pixel of the scene into one of 16 classes (alfalfa, corn-notill, corn-mintill, corn, grass-pasture, grass-trees, grass-pasture-mowed, hay-windrowed, oats, soybean-notill, soybean-mintill, soybean-clean, wheat, woods, buildings-grass-trees-drives, stone-steel-towers). For training the network, we use the spectral bands from $s = 1000$ randomly chosen pixel points, $y_k \in \mathbb{R}^{220}$, $k = 1, \ldots, s$, together with their corresponding class probability vectors $c_k \in \mathbb{R}^{16}$ (unit vectors). The goal is to predict the correct classes of new pixel points in the scene (Figure 5).

We use a ResNet architecture with ReLU activation (i.e. $\sigma(x) = \max\{0, x\}$, smoothed around zero) and define the linear operations $K(\cdot)$ at each layer to be a dense matrix representation of the weights $\theta$. We choose a network depth of $T = 20$ discretized with up to $N = 2048$ layers and a network width of 220 channels.

3. MNIST image classification (MNIST)

As a final example, we consider the now classic MNIST test case for classification of hand-written digits encoded in a $28 \times 28$ grey scale image [44]. Our objective for this test case is to demonstrate the scalability of the layer-parallel approach over an increasing number of layers. While we obtain reasonable validation accuracy, the objective is not to develop an optimal ResNet to solve this problem. Further, we obtained the timings below with our own straight-forward implementation of convolutions, to ensure compatible layer-to-layer propagators with XBraid for our initial tests. Future work will use a fast convolution library, which will provide a substantial speedup to both the serial and layer-parallel codes.

We use a ResNet architecture with tanh activation and define internal layers by the linear operator $K(\cdot)$ using 8 convolution kernels of width 3. This yields a weight tensor at each layer of size $\mathbb{R}^{3\times3\times8\times8}$. The parameters to be trained are $\mathbb{R}^{28\times28}$ at each layer. The opening layer,
provides a replication of the original image to the 8 convolutions with an applied activation (there are no weights in the opening layer). A final classification layer is applied that takes the 8 convolutions using a dense $K(\cdot)$ to the 10 classes associated with MNIST. The internal layers are defined to have a network depth of $T = 5$ with up to $N = 2048$ layers.

For all cases, the optimization objective function consists of the softmax loss function, plus a Tikhonov-regularization term for $\theta, W$ and $\mu$, as well as an additional regularization term for $\theta$ that enforces smoothness across the network layers. The computations for the MNIST results were performed on the Skybridge capacity cluster at Sandia National Laboratories. Skybridge is a Cray containing 1848 nodes with two 8 core Intel 2.6 GHz Sandy Bridge processors, 64GB of RAM per node and an Infiniband interconnect.

5.2 Layer-parallel scaling and performance validation

First, we compare the performance of the layer-parallel MGRIT approach for forward and backward propagation to a layer-serial implementation. We consider one objective function and gradient evaluation for fixed network weights using a batch of examples of sizes $s = 5000, 1000, 500$ for the peaks, indian pines and MNIST test case, respectively. We choose a coarsening factor of $c = 4$ to set up a hierarchy of ever coarser layer grids to employ the multigrid scheme.

Figure 6 shows the convergence history of the MGRIT iterations for two different problem sizes using $N = 256$ and $N = 1024$ layers. Here, we monitor the relative drop of the state and adjoint residual norms during the MGRIT iterations. It proves fast convergence for all test cases and independent of the number of layers.

Figure 7 presents a weak-scaling study for the layer-parallel MGRIT iterations. Here, we double the number of layers as well as the number of compute cores while keeping the ratio $N/#\text{cores} = 4$ fixed, such that each compute unit processes 4 layers. Runtimes are measured for one objective function and gradient evaluation with the layer-parallel MGRIT approach, using a relative stopping criterion for the MGRIT residual norms of 5 orders of magnitude. Note, that the layer-serial data points have been added for comparison, even though they are executed on only one core. For the layer-serial propagation, doubling the number of layers leads to a doubling in runtime. The layer-parallel MGRIT approach however yields nearly constant runtimes independent of the problem size. The resulting speedups are reported in Table 1. Since the layer-parallel MGRIT approach
Figure 6: Convergence history of MGRIT solving the state and adjoint equations for $N = 256$ and $N = 2048$ layers.
removes the linear runtime scale of the conventional serial-layer propagation, resulting speedups increase linearly with the problem size yielding up to a factor of 18x for the MNIST case using 2048 layers and 512 cores. Further speedup can be expected when considering ever more layers (and computational resources).

A strong scaling study for all test cases is presented Figure 8 for various numbers of layers. Here, we keep the problem sizes fixed and measure the time-to-solution for one gradient evaluation with MGRIT for increasing numbers of computational resources. It shows good strong scaling behavior for all test cases, independent of the numbers of layers. The cross over point where the layer-parallel MGRIT approach shows speedup over the layer-serial propagation is around 16 cores for all cases (compare with the layer-serial runtimes from Table 1).

5.3 Simultaneous layer-parallel training validation

We investigate the simultaneous layer-parallel training for the Peaks and Indian Pines test cases, performing $m_1, m_2 = 2$ layer-parallel MGRIT iterations in each outer training iteration. For the Peaks example, we train a network with $N = 1024$ layers distributed onto 256 compute cores and for the Indian Pines data set, we choose $N = 512$ layers distributed onto 128 compute cores, giving
<table>
<thead>
<tr>
<th>Testcase</th>
<th>$N$</th>
<th>#Cores</th>
<th>Layer-parallel</th>
<th>Layer-serial</th>
<th>Speedup</th>
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</thead>
<tbody>
<tr>
<td>Peaks</td>
<td>256</td>
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<td>1.8 sec</td>
<td>1.8</td>
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<tr>
<td></td>
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<td>128</td>
<td>1.4 sec</td>
<td>3.7 sec</td>
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<td>8.1</td>
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<tr>
<td>Indian</td>
<td>256</td>
<td>64</td>
<td>1.3 min</td>
<td>2.6 min</td>
<td>2.0</td>
</tr>
<tr>
<td>Pines</td>
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<td>1.5 min</td>
<td>5.2 min</td>
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<td></td>
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<td>6.1</td>
</tr>
<tr>
<td></td>
<td>2048</td>
<td>512</td>
<td>2.0 min</td>
<td>20.8 min</td>
<td>10.3</td>
</tr>
<tr>
<td>MNIST</td>
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<td></td>
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<td></td>
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<td>512</td>
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<td>36.6 min</td>
<td>16.0</td>
</tr>
</tbody>
</table>

Table 1: Runtime speedup of layer-parallel gradient evaluation over layer-serial propagation.

![Graphs](a) Peaks example (b) Indian Pines (c) MNIST

Figure 8: Strong scaling study for a layer-parallel gradient evaluation for various problem sizes from $N = 256$ to $N = 2048$ layers. The cross-over point where the layer-parallel approach yields speedup over the layer-serial propagation lies around 16 cores (compare to Table 1).
4 layers per processor in both test cases. We compare runtimes of the simultaneous layer-parallel training with a conventional layer-serial training approach, while choosing the same preconditioning Hessian approximation (L-BFGS), as well as the same initial network parameters for both approaches. However, we tune the optimization hyper-parameters (such as regularization parameters, stepsize selection, etc.) separately for both schemes, in order to find the best setting for either approach that reaches a prescribed validation accuracy with least iteration counts and minimum runtime.

Figure 9 plots the training history for the layer-parallel simultaneous optimization approach compared to a conventional layer-serial training approach. We validate from the top figures, that both approaches reach comparable performance in terms of training result (optimization iteration counts, training loss and validation accuracy). Hence, reducing the accuracy of the inner multigrid iterations for solving the state and adjoint equations within a simultaneous training framework does not deteriorate the training behavior. But, each iteration of the simultaneous layer-parallel approach is much faster than for the layer-serial approach due to the layer-parallelization and the reduced state and adjoint accuracy. Therefore, the overall runtime for reaching that same final training result is reduced drastically (bottom figures). Runtime speedups are reported in Table 2. We observe a speedup of 6.0 for the Peaks example when using 256 cores, which is a parallel efficiency of about 2.3%. In the larger Indian Pines example, the reported speedup of 4.4 using 128 cores gives a parallel efficiency of 3.4%. This reduces the time-to-solution from about 45 hours to about 10 hours. While these results have been computed for selected fixed $N$, it is expected that the speedup scales linearly with increasing numbers of layers, similar to the observation in Table 1.

<table>
<thead>
<tr>
<th>Test case</th>
<th>$N$</th>
<th>#Cores</th>
<th>Layer-parallel</th>
<th>Layer-serial</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
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<td>683 sec</td>
<td>4096 sec</td>
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<td>Indian Pines</td>
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<td>128</td>
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<td>2623 min</td>
<td>4.4</td>
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</table>

Table 2: Runtime speedup of simultaneous layer-parallel training over layer-serial training.

6 Conclusion

In this paper, we provide a proof-of-concept for layer-parallel training of deep residual neural networks (ResNets). The similarity of training ResNets to the optimal control of nonlinear time-dependent differential equations motivate us to use parallel-in-time methods that have been popular in many engineering applications. The method developed is based on nonlinear multigrid methods and introduces a new form of parallelism across layers.

We demonstrate two options to benefit from the layer-parallel approach. First, the nonlinear multigrid reduction in time (MGRIT) method can be used to replace forward and backward propagation in existing training algorithms, including for stochastic approximation methods such as SGD. In our experiments, this leads to speedup over serial implementations when using more than 16 compute nodes. Second, additional savings can be obtained through the simultaneous layer-parallel training, which uses only inexact forward and backward propagations.

While the reported speedups might seem small in terms of parallel efficiency, these reductions can be of significant importance when considering large overall training runtimes. When bare training runtimes are in the order of days, any runtime reduction is appreciated, as long as compu-
Figure 9: Training loss (solid lines) and validation accuracy (dashed lines) over training iterations (top) and compute time (bottom). For the layer-parallel training, each core processes 4 layers. The simultaneous layer-parallel approach reaches training results comparable to a layer-serial approach within much less computational time.

Motivated by these first promising results, we will investigate the use of layer-parallel training for more challenging learning tasks, including more complex image-recognition problems. Further reducing the memory footprint of our algorithm in those applications motivates the use of reversible networks arising from hyperbolic systems [14]. A challenge arising here is the interplay of MGRIT and hyperbolic systems.
References


