OPTIMIZING MGRIT AND PARAREAL COARSE-GRID OPERATORS FOR LINEAR ADVECTION

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Abstract. Parallel-in-time methods, such as multigrid reduction-in-time (MGRIT) and Parareal, provide an attractive option for increasing concurrency when simulating time-dependent PDEs in modern high-performance computing environments. While these techniques have been very successful for parabolic equations, it has often been observed that their performance suffers dramatically when applied to advection-dominated problems or purely hyperbolic PDEs using standard rediscretization approaches on coarse grids. In this paper, we apply MGRIT or Parareal to the constant-coefficient linear advection equation, appealing to existing convergence theory to provide insight into the typically non-scalable or even divergent behaviour of these solvers for this problem. To overcome these failings, we replace rediscretization on coarse grids with near-optimal coarse-grid operators that are computed by applying optimization techniques to approximately minimize error estimates from the convergence theory. Our main finding is that, in order to obtain fast convergence as for parabolic problems, coarse-grid operators should take into account the behaviour of the hyperbolic problem by tracking the characteristic curves. Our approach is tested on discretizations of various orders that use explicit or implicit Runge-Kutta time integration with upwind-finite-difference spatial discretizations, for which we obtain fast and scalable convergence in all cases. Parallel tests also demonstrate significant speed-ups over sequential time-stepping. Additionally, results indicate that parallel-in-time integration is more effective for higher-order discretizations of this problem than for those of low order. Our insight of tracking characteristics on coarse grids is implemented for linear advection using an optimization approach, but the principle is general, and provides a key idea for solving the long-standing problem of efficient parallel-in-time integration for hyperbolic PDEs.

Key words. Multigrid, MGRIT, Parareal, parallel-in-time, hyperbolic, high-order

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1. Introduction. Parallelism in the context of the large-scale numerical simulation of time-dependent partial differential equations (PDEs) has historically been limited to the spatial aspect of these problems, with the temporal integration being handled sequentially. Due to the stagnation of processor clock speeds, we have seen the advent of massively parallel machines, of which the largest currently have millions of cores. On these machines, spatial parallelism alone tends to saturate quickly due to communication overheads and, so, faster compute times necessitate the use of algorithms with greater concurrency. A promising strategy for increasing concurrency is the use of parallel-in-time methods, which introduce parallelism into the temporal direction. These algorithms have seen a large amount of interest over the last two decades, as described in the review by Gander [14].
Two of the most well-known parallel time integration methods are Parareal [22] and multigrid reduction-in-time (MGRIT) [8], which can both be considered as multigrid methods, although Parareal also has other interpretations [16]. For a wide variety of diffusion-dominated problems, these algorithms can achieve a significant reduction in wall clock time over sequential time-stepping methods, given enough parallel resources [8–11]. Despite their success for diffusion-dominated problems, MGRIT and Parareal (along with most other parallel-in-time methods) tend to perform quite poorly on hyperbolic PDEs. More generally, they typically exhibit extremely slow convergence or even divergence\(^1\) when applied to advection-dominated PDEs [4,5,7,13,16,17,20,21,23–26,29]. Moreover, many of these examples demonstrate a clear deterioration in convergence as the amount of dissipation in the underlying PDE and/or its discretization is decreased [20,26,29].

There are only a few documented cases in the literature where effective MGRIT or Parareal strategies have been applied to advection-dominated equations. Several so-called ‘stabilized’ variants of Parareal have been developed [4, 5, 25]. While these methods improve upon the convergence of standard Parareal applied to hyperbolic problems, they are often significantly more expensive per iteration than the original algorithm, and so their practicability is limited. The use of semi-Lagrangian coarse-grid operators was considered in [26], inspiring some of the work in this paper. Unfortunately, though, the approach in [26] showed significantly degraded convergence as diffusion was eliminated from the PDE in question. In particular, iteration counts needed for convergence increased from about five when diffusion was significant to about 25 in the hyperbolic/no-diffusion limit, representing one quarter of the number of iterations required to achieve the exact solution.

In [23], speed-up was obtained for a high-order accurate discretization of the shallow water equations, but the approach employed a low-order method as the coarse time integrator which avoids the coarse-grid issues for MGRIT that are the central topic of this paper. Linear advection and Burgers’ equations where considered in [21], where, to provide both cheaper multigrid cycles and overcome stability issues arising from coarsening only in time, coarsening in space was also used. While [21] demonstrated parallel speed-up, convergence was, ultimately, slow and not scalable, and the approach did not work when applied to higher than first-order discretizations. More generally, where speed-ups have been reported for hyperbolic PDEs in the literature, they are typically quite small, being on the order of two to six times faster than that of sequential time-stepping, with slow convergence of the iteration ultimately inhibiting faster runtimes due to increased parallelism. For comparison, in [11], a speed-up on the order of 20 times was achieved for a diffusion-dominated parabolic problem.

A number of theoretical convergence analyses have been developed for Parareal and MGRIT [6, 7, 12, 15, 16, 18, 24, 28], which have helped to explain numerical convergence results, and will likely play an important role in the design of new solvers. Furthermore, some theoretical studies have identified potential roadblocks for fast parallel-in-time convergence of hyperbolic PDEs [13, 16]. Nevertheless, there does not yet exist a general understanding of why parallel time integration of advection-

\(^1\)Note that both MGRIT and Parareal are known to converge to the exact solution of the discrete problem after a finite number of iterations [8], due to sequential propagation of the initial condition across the temporal domain by the relaxation scheme. As such, in this paper, we use the term ‘divergence’ to describe solvers that converge to the solution only in a number of iterations close to that for which they would reach the exact solution, which is typically accompanied by a large initial growth in the approximation error, similar to that seen in diverging spatial multigrid (or other) iterations.
dominated problems seems to be so much more difficult than for their diffusion-dominated counterparts. For example, efficient parallel-in-time solvers for the constant-coefficient linear advection problem—arguably the simplest of all hyperbolic PDEs—have not yet been developed, with typical approaches not being scalable, exhibiting extremely slow convergence, or diverging altogether [7,20,21].

The aim of this paper is to demonstrate that, in fact, MGRIT and Parareal, with the right choice of coarse-grid operator, can efficiently integrate hyperbolic PDEs despite previous results that had put this in doubt [13,16]. To do so, we work in an idealised environment, whereby we consider the constant-coefficient linear advection problem in one spatial dimension subject to periodic spatial boundary conditions, such that we can appeal to existing sharp MGRIT convergence theory. Informed by convergence theory and the PDE, we develop heuristics that coarse-grid operators should satisfy and we formulate optimization problems based on these to find ‘near-optimal’ coarse-grid operators. For example, one such heuristic that we have adopted (after failing to obtain satisfactory results using standard approaches) is that coarse-grid operators should track information along characteristics akin to the semi-Lagrangian schemes considered in [26]. We demonstrate that our near-optimal coarse-grid operators lead to fast and scalable convergence, in just a handful of iterations for both implicit and explicit discretizations, resulting in significant speed-ups in parallel over sequential time-stepping, which is comparable to what has been achieved for parabolic PDEs. Notably, our results include the use of high-order accurate discretizations (up to fifth order), which is important because many results reported in the literature for hyperbolic PDEs have used diffusive, low-order discretizations that have likely aided the convergence of the given parallel-in-time method. Additionally, our approach works for large coarsening factors, and we employ fine-grid CFL numbers that reflect what would realistically be used with sequential time-stepping. This stands in contrast to many existing results in the literature, where unrealistically small fine-grid CFL numbers are needed to obtain convergent solvers.

The optimization approaches presented in this paper rely on analytical operations and computational optimizations that are feasible specifically for the case of one-dimensional, constant-coefficient linear advection. This precludes direct application of these approaches to more complicated hyperbolic PDEs. Crucially, though, they give us powerful tools to demonstrate that, for this canonical hyperbolic PDE, it is possible to obtain highly efficient MGRIT and Parareal solvers, but only if one uses coarse-grid operators that track information along characteristics. At the same time, our main finding that coarse-grid operators should track characteristics is general, and we believe it will prove relevant to the design of coarse-grid operators for more complicated hyperbolic PDEs. Practical methods for selecting coarse-grid operators for linear advection and other hyperbolic problems that follow this main insight are the subject of further research.

The remainder of this paper is organized as follows. In §2, the model problem and its discretizations are introduced, a brief overview of MGRIT and Parareal is given, and some motivating numerical examples are presented. A general discussion on convergence theory and what it reveals about the difficulty of hyperbolic problems is given in §3. Section 4 develops linear least squares algorithms for finding near-optimal coarse-grid time-stepping operators for the model problem. Parallel results are given in §5 for some of the newly developed coarse-grid operators. Concluding remarks and a discussion of future work is the subject of §6.
2. Preliminaries. In this section, we outline the model problem, its discretizations, and give a brief summary of MGRIT and Parareal. We then demonstrate the difficulty our seemingly simple model problem poses for these algorithms via some numerical examples.

2.1. Model problem and discretizations. For our model problem, we consider the one-dimensional linear advection equation,

\[ \frac{du}{dt} + \alpha u_x = 0, \quad (x, t) \in [0, L] \times (0, T_f], \quad u(x, 0) = \sin^4(\pi x), \tag{2.1} \]

with constant wave speed \( \alpha > 0 \). While the exact solution of this canonical hyperbolic PDE is just the shifted initial condition, and its numerical approximation is easily obtained in the sequential time-marching setting, it presents enormous difficulty for parallel-in-time solvers. In what follows, we consider periodic boundary conditions in space and, in Supplementary Material SM2, we demonstrate that our approach can be extended successfully to inflow/outflow boundaries.

To numerically approximate the solution of (2.1), finite-difference spatial discretizations are used with Runge-Kutta time integrators. As such, the spatial domain \( x \in [-1, 1] \) is discretized with \( n_x + 1 \) equidistant points with spacing \( \Delta x \), and the temporal domain \( t \in [0, T_f] \) is discretized with \( n_t + 1 \) equidistant points having a spacing of \( \Delta t \). We employ the method of lines to generate a semi-discretized representation. First, a \( p \)-th order upwind finite-difference spatial discretization is applied to (2.1), resulting in the system of ordinary differential equations (ODEs)

\[ \frac{d u}{d t} = \mathcal{L} u, \quad t \in (0, T_f], \quad u(0) = u(x, 0), \tag{2.2} \]

in which \( \mathcal{L}: \mathbb{R}^{n_x} \rightarrow \mathbb{R}^{n_x} \) represents the discretization of \(-\alpha \partial_x u \) on the spatial mesh. Since \( \alpha \) is constant and periodic boundaries are applied, \( \mathcal{L} \) is a circulant matrix and is, thus, unitarily diagonalized by the discrete Fourier transform (DFT). Specifically, we use upwind-finite-difference spatial discretizations of orders 1–5, which we denote as U1–U5, given by

(U1) \[ u'(x_i) = \frac{1}{\Delta x} [u_{i} - u_{i-1}] + \mathcal{O}(\Delta x), \]

(U2) \[ u'(x_i) = \frac{1}{2\Delta x} \left[ 3u_{i} - 4u_{i-1} + u_{i-2} \right] + \mathcal{O}(\Delta x^2), \]

(U3) \[ u'(x_i) = \frac{1}{6\Delta x} \left[ 2u_{i+1} + 3u_{i} - 6u_{i-1} + u_{i-2} \right] + \mathcal{O}(\Delta x^3), \]

(U4) \[ u'(x_i) = \frac{1}{12\Delta x} \left[ 3u_{i+1} + 10u_{i} - 18u_{i-1} + 6u_{i-2} - u_{i-3} \right] + \mathcal{O}(\Delta x^4), \]

(U5) \[ u'(x_i) = \frac{1}{60\Delta x} \left[ -3u_{i+2} + 30u_{i+1} + 20u_{i} - 60u_{i-1} + 15u_{i-2} - 2u_{i-3} \right] + \mathcal{O}(\Delta x^5). \]

The odd-order discretizations have a one-point bias, and those with even-order have a two-point bias. To construct a \( p \)-th order spatial discretization, \( p + 1 \) nodes are selected and then the weights are uniquely determined using well-known techniques, as described in [27], for example.

The ODE system (2.2) is then discretized using either a \( p \)-th order explicit Runge-Kutta (ERK) method, or a \( p \)-th order, L-stable singly diagonally implicit Runge-Kutta (SDIRK) method, with the resulting scheme denoted as either ERK\( p+U_p \), or SDIRK\( p+U_p \). We consider ERK schemes of orders 1–5, of which orders 1–4 have
1–4 stages, and the 5th-order scheme has 6 stages. The specific ERK schemes used are as follows: The 1st-order scheme is Euler’s method; the 2nd- and 3rd-order methods are the ‘optimal’ strong-stability-preserving schemes [19, (9.7), (9.8)]; the 4th-order scheme is the ‘classical Runge-Kutta method’ [2, p. 180]; and finally, see [2, (236a)] for the 5th-order scheme. For SDIRK schemes, orders 1–4 are considered, with orders 1–3 having 1–3 stages, and the 4th-order scheme having 5 stages. The first-order scheme is simply Euler’s method; the 2nd- and 3rd-order methods can be found in [2, pp. 261–262]; and the 4th-order scheme is given by [32, (6.16)]. Butcher tableaus for these Runge-Kutta schemes can be found in Supplementary Material SM1.

Upon application of a Runge-Kutta scheme to ODEs (2.2), their numerical solution may be written in the one-step form

\[ u^{n+1} = \Phi u^n, \quad u^0 = u(0), \quad n = 0, \ldots, n_t. \] (2.3)

Note that equations (2.3) can be written as a single, large space-time block lower bidiagonal linear system. Here, \( \Phi : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}^{n \times n} \) is known as the ‘time-stepping operator,’ as it steps the discrete solution from one time level to the next. The eigenvalues of \( \Phi \) can be computed as function of those of \( L \) [7, 18]. In fact, it can be shown that \( \Phi \) is a rational function (in a matrix sense) of \( L \), as in Lemma 2.1.

**Lemma 2.1 (Rational form of \( \Phi \)).** Let \( R(z) = P(z)/Q(z) \) denote the stability function [2, lemma 351A] of a Runge-Kutta scheme applied to (2.2), in which \( P \) and \( Q \) are polynomials derived from the Butcher tableau of the scheme. Then, for diagonalizable matrices \( L \in \mathbb{R}^{n \times n} \), the time-stepping operator in (2.3) is

\[ \Phi(\Delta t L) = P(\Delta t \xi_k)\{Q(\Delta t \xi_k)\}^{-1}. \] (2.4)

**Proof.** Let \( X \) denote the matrix having eigenvectors of \( L \) as its columns. Substituting \( u = Xv \) into (2.2) and left multiplying by \( X^{-1} \) yields a system of \( n_x \) decoupled ODEs of the form \( \frac{dv_k}{dt} = \xi_k v_k, \ k = 1, \ldots, n_x, \) in which \( \xi_k \) is the \( k \)th eigenvalue of \( L \). Using the Runge-Kutta stability function, the one-step numerical solution of the \( k \)th component of the decoupled ODEs is \( v_k^{n+1} = R(\Delta t \xi_k)v_k^n = P(\Delta t \xi_k)/Q(\Delta t \xi_k)v_k^n. \) The one-step solution of the system of decoupled ODEs can then be written as \( v^{n+1} = P(\Delta t \text{diag}(\xi))(Q(\Delta t \text{diag}(\xi)))^{-1}v^n. \) Making the substitution \( v = X^{-1}u \), left multiplying by \( X \), and noting \( XG(\Delta t \text{diag}(\xi)) X^{-1} = G(\Delta t \text{diag}(\xi)) X^{-1} = G(\Delta t L) \) for any rational function, \( G \), yields the result.

For an ERK scheme, \( Q(z) = 1 \) and so the Runge-Kutta stability function used in Lemma 2.1 is simply a polynomial, \( R(z) \equiv P(z) \).

**Corollary 2.2.** For periodic boundary conditions applied to (2.1), the time-stepping operator \( \Phi \) in (2.3) can be written as the product of a sparse circulant matrix and the inverse of a sparse circulant matrix. In the case of an ERK scheme, \( \Phi \) is simply a sparse circulant matrix.

**Proof.** For periodic boundaries, the finite-difference spatial discretizations \( L \) are sparse and circulant, and noting that circulant matrices are closed under addition and multiplication, the result follows immediately from the rational form of \( \Phi \) in (2.4).

The CFL number for Runge-Kutta finite-difference discretizations of (2.1) is defined as

\[ c := \alpha \frac{\Delta t}{\Delta x}. \] (2.5)
The explicit discretizations considered here suffer from a CFL limit, for which a necessary condition for numerical stability is \( c \leq c_{\text{max}} \). Values of \( c_{\text{max}} \) can be computed from the Runge-Kutta stability function and the eigenvalues of \( \Delta t \mathcal{L} \), and are given in Table 1. Throughout the remainder of this paper, experiments using ERK discretizations will employ a CFL fraction—ratio of CFL number to CFL limit—of 85%, \( c = 0.85c_{\text{max}} \). A value of 85% has been (somewhat arbitrarily) chosen since it is a significant fraction of a scheme’s CFL limit and, so, it is realistic of what would be used for regular time-stepping. In all SDIRK experiments, a CFL number of \( c = 4 \) is used. All of the SDIRK+U schemes considered here are unconditionally stable since the real components of the eigenvalues of the circulant matrices \( \Delta t \mathcal{L} \in \mathbb{R}^{n_x \times n_x} \) are non-positive independently of \( n_x \), which means they lie in the stability region of any L-stable Runge-Kutta method.

| Scheme | ERK1+U1 | ERK2+U2 | ERK3+U3 | ERK4+U4 | ERK5+U5 |
|--------|---------|---------|---------|---------|---------|
| \( c_{\text{max}} \) | 1       | 1/2     | 1.62589... | 1.04449... | 1.96583... |

To demonstrate the accuracy of the discretizations used here and to emphasize that the high-order methods faithfully represent the non-dissipative nature of (2.1), computed discretization errors are shown in Figure 1.

Fig. 1. Space-time discretization errors for (2.1) measured in the discrete \( L_2 \)-norm. Left: ERK+U with ERK\( p \)+U\( p \) using a final integration time of \( T_f \approx \{6.8, 6.8, 5.5, 7.1, 6.7\} \) for \( p \in \{1, 2, 3, 4, 5\} \). Right: SDIRK+U with \( T_f = 8 \). Anchored near the final measurement for each discretization is a dashed line showing the theoretical convergence rate of each scheme (order \( p \) for ERK\( p \)/SDIRK\( p \)+U\( p \)). Note the use of different scalings of the vertical axes in the two plots to better highlight the data within each plot.

### 2.2. MGRIT, Parareal, and numerical set-up.

The purpose of this section is to give a brief overview of MGRIT and Parareal, and describe the set-up for our numerical tests. MGRIT and Parareal are parallel, multilevel, iterative methods for solving block lower triangular systems arising from evolutionary problems, such as (2.3); note, however, that Parareal is typically only thought of as a two-level method. In this paper, we make no significant differentiation between MGRIT and Parareal, since Parareal can be described in the MGRIT framework via certain choices of algorithmic parameters (as discussed below). As such, beyond the current section, we will refer collectively to these algorithms as MGRIT.
We now give an overview of the MGRIT algorithm as it applies to model problem (2.3); see [7, 8] for more detailed descriptions. The temporal mesh \((t^n)_{n=0}^{n_t} := (n\Delta t)_{n=0}^{n_t}\) on which the problem is posed is the ‘fine grid,’ and an integer coarsening factor \(m > 1\) is used to induce a ‘coarse grid’ consisting of a subset of the fine-grid points, \((mn\Delta t)_{n=0}^{n_t/m}\). The set of points appearing exclusively on the fine grid are called ‘F-points,’ while those appearing on both fine and coarse grids are ‘C-points.’ An MGRIT iteration combines pre-relaxation with a coarse-grid correction. The two fundamental types of relaxation are: F-relaxation, which is time-stepping starting from each C-point across the following F-interval; and C-relaxation, which is time-stepping from the last F-point in each interval to its following C-point. The standard relaxation sweeps performed in MGRIT are either: F-relaxation (Parareal uses F-relaxation almost exclusively), or the stronger FCF-relaxation, which is an F-, followed by a C-, followed by an F-relaxation.

The coarse-grid problem is obtained by approximating the Schur complement system (with respect to C-points) of the fine-grid residual equation. This results in the algebraic error \(e_c\) at C-points being approximated by the block lower-bidiagonal system

\[
\begin{align*}
  e_c^{n+1} &= \Psi e_c^n + r_c^{n+1}, & e_c^0 &= 0, & n = 0, \ldots, n_t/m - 1,
\end{align*}
\]  

(2.6)

in which \(r_c^{n+1}\) is the fine-grid residual at the \(n + 1\)st C-point, and \(\Psi : \mathbb{R}^{n_x} \to \mathbb{R}^{n_x}\) is the coarse-grid time-stepping operator, responsible for propagating the error from one C-point to the next. After solving (2.6), the coarse-grid error is interpolated to the fine grid via so-called ‘ideal interpolation’ which corresponds to injection at C-points followed by an F-relaxation. To solve coarse-grid problem (2.6), one can either do a sequential forward solve, or recursively apply the algorithm since (2.6) has the same block lower-bidiagonal structure as fine-grid problem (2.3). A sequential coarse-grid solve is almost always used in Parareal algorithms, making them two-level solvers.

The above algorithm can be generalised to accommodate more complicated problems, such as those using spatial coarsening, or those with nonlinearities [11,21].

Taking \(\Psi = \Psi_{\text{ideal}} := \Phi^m\) defines an ideal coarse-grid time-stepping operator in the sense that the exact solution of (2.3) is reached in a single MGRIT iteration. In this instance, coarse-grid problem (2.6) really is the Schur complement system of the fine-grid residual equation. However, no speed-up in parallel can be achieved with \(\Psi = \Psi_{\text{ideal}}\) since the sequential coarse-grid solve is as expensive as the original problem of time-stepping with \(\Phi\) across the entire fine grid. Instead, one should choose \(\Psi\) to be some approximation of \(\Phi^m\)—or equivalently, it should approximate taking \(m\) steps with \(\Phi\) on the fine grid—under the constraint that its action is significantly cheaper to compute so that speed-up can be achieved. Typically \(\Psi\) is chosen through the process of rediscretizing \(\Phi\) on the coarse grid; that is, by using the fine-grid discretization with the enlarged coarse-grid time step, \(m\Delta t\) [6–8]. Other techniques, such as coarsening in the order of the discretization have also been applied [10,23].

The primary objective of this paper is to develop near-optimal coarse-grid operators, \(\Psi\), for discrete model problem (2.3) deriving from advection problem (2.1). For explicit temporal discretizations of the model problem, \(\Phi\) and \(\Psi_{\text{ideal}} := \Phi^m\) are sparse, circulant matrices (Corollary 2.2), and based on this, in §4, we develop coarse-grid operators, \(\Psi\), that are also sparse, circulant matrices. To ensure computing the action of \(\Psi\) is less expensive than that of \(\Psi_{\text{ideal}}\), we place restrictions on its sparsity. For implicit discretizations, the situation is more complicated as \(\Phi\) and \(\Psi_{\text{ideal}}\) are rational functions of sparse, circulant matrices. However, in §4.5, we show that using sparse coarse-grid operators is appropriate in some situations.
For definiteness, we now describe all of the settings used in our numerical experiments. The initial iterate for the space-time solution is taken to be uniformly random except at the initial time, where it matches the prescribed initial condition. Unless otherwise noted, the metric used to report solver convergence is the number of iterations needed to achieve a space-time residual below $10^{-10}$ in the discrete $L_2$-norm. Note that with the random initial iterate, the initial discrete $L_2$-norm of the space-time residual is $O(1)$, and so this convergence criterion is roughly equivalent to reducing the initial residual norm by 10 orders of magnitude. This stopping criterion exceeds the accuracy of the underlying discretizations in almost all cases, and so its use typically leads to a dramatic ‘over solving’ of the space-time system with respect to the discretization error. Nonetheless, we use such a small halting tolerance to highlight the asymptotic convergence behaviour of the solvers we develop. For all ERK\(p+U\) tests, a spatial resolution is selected, and a number of points $n_t$ in time is chosen to be the largest power of two such that $\Delta t n_t$ does not exceed 8. For $p \in \{1, 2, 3, 4, 5\}$, this results in final integration times $T_f \approx \{6.8, 6.8, 5.5, 7.1, 6.7\}$. For all SDIRK+U tests, $T_f = 8$ and $n_t = n_x$ such that a CFL number (2.5) of $c = 4$ results. Where scaling tests are presented, the mesh is refined uniformly in both space and time such that the CFL number of the fine-grid discretization remains constant.

2.3. Failure of MGRIT with rediscretization for the model problem.
To provide a baseline for the numerical results shown in the later sections of this paper, we now present some numerical results for model problem (2.1) using MGRIT with rediscretized coarse-grid operators. For all ERK+U discretizations of (2.1), the use of a rediscretized coarse-grid operator leads to divergent solvers for all coarsening factors $m$. This behaviour is driven primarily by a CFL-type instability: For coarsening factors $m > 1$, the coarse-grid CFL limit is violated (recalling fine-grid CFL numbers are set to 85% of their respective limits), and so the coarse-grid solution is numerically unstable and, hence, cannot feasibly be used to accelerate convergence to the (stable) fine-grid solution. To overcome this instability, one possible strategy is to couple the explicit fine-level discretization with a stable, implicit coarse-grid discretization. In such cases, a large coarsening factor needs to be employed to amortize the much larger cost of solving an implicit coarse-grid problem. However, this technique seldom results in a good solver (again, it is usually divergent) because the approximation it provides to $\Psi_{\text{ideal}} := \Phi^m$ is simply not good enough, even for small $m$. In the few instances where parallel speed-up has been achieved for explicit discretizations of hyperbolic problems, alternative techniques have been used, such as incorporating spatial coarsening [21], or coarsening in the order of the discretization without coarsening in time [23]. Thus, we do not present numerical results for ERK discretizations here because the standard multigrid-in-time choice of rediscretization is divergent and, to the best of our knowledge, there is no other technique for developing efficient coarse-grid operators of hyperbolic problems for use in these time-only coarsening algorithms.

In contrast to explicit discretizations, unconditionally stable, implicit fine-grid discretizations can be rediscretized on coarse grids to provide stable coarse-grid operators. Two-level MGRIT iteration counts for SDIRK+U discretizations of (2.1) using such a rediscretized coarse-grid operator are given in the left side of Table 2. All solvers, with the exception of SDIRK1+U1 are divergent in the sense that they converge to the prescribed tolerance in approximately $n_t/(2m)$ iterations (shown in the right side of the table). This is the number of iterations for which they exactly achieve the sequential time-marching solution, which means that each parallel proces-
Sor does more work than a sequential processor would to solve the whole problem. Notice that some solves have required slightly more than the $n_t/(2m)$ iterations for which the exact solution should have been obtained. This is a consequence of using finite-precision arithmetic: The ability to achieve the exact solution in $n_t/(2m)$ iterations is limited by the conditioning of $\Phi$ and the size of the error relative to the solution as the algorithm proceeds. The relatively good—but still poor—performance of SDIRK1+U1 is attributable to the fact that it is highly diffusive (see Figure 1), and does not represent the non-dissipative behaviour of (2.1) well.

Note that MGRIT convergence rates for implicit discretizations of hyperbolic problems are dependent on the CFL number, with smaller CFL numbers typically resulting in faster convergence, just as in the explicit case, even though there is no CFL limit to be violated. This can be can be seen by contrasting the types of convergence rates reported in [7] for linear advection with those shown in Table 2 for more realistic CFL numbers. The results of Table 2 exemplify just how poorly MGRIT performs for hyperbolic problems when using rediscretized coarse-grid operators. This is especially evident when contrasted with results for model diffusion-dominated problems where convergence is typically achieved within 10 or so iterations, even for high-order discretizations and large coarsening factors [7,8].

| Scheme       | $n_x \times n_t$     | $m$ (measured) | $m$ (exact) |
|--------------|---------------------|----------------|-------------|
| SDIRK1+U1    | $2^{10} \times 2^{10}$ | 18             | 256         |
|              | $2^{12} \times 2^{12}$ | 18             | 1024        |
| SDIRK2+U2    | $2^{10} \times 2^{10}$ | 40             | 128         |
|              | $2^{12} \times 2^{12}$ | 241            | 1024        |
| SDIRK3+U3    | $2^{10} \times 2^{10}$ | 1008           | 256         |
|              | $2^{12} \times 2^{12}$ | 183            | 1024        |
| SDIRK4+U4    | $2^{10} \times 2^{10}$ | 891            | 256         |
|              | $2^{12} \times 2^{12}$ | $\times$       | 520         |

3. Convergence theory applied to hyperbolic problems. To better understand the origins of the poor convergence of MGRIT applied to the model problem (as shown in the previous section), and hyperbolic PDEs more generally, we now recall the two-level MGRIT convergence theory from [7] and discuss some of its implications for hyperbolic problems.

3.1. Two-level convergence theory. The convergence behaviour of MGRIT can be understood by analysing its error propagation matrix. Let $T$ denote such a matrix, and let the initial space-time error be $e^{(0)}$. Then, after $q$ MGRIT iterations, the error obeys $\|e^{(q)}\| = \|T^q e^{(0)}\| \leq \|T^q\|\|e^{(0)}\| = \|T\|^q \|e^{(0)}\|$. Due to the nilpotency of $T$, the short term convergence behaviour of the algorithm is more accurately reflected by its norm rather than its spectral radius, which is zero because the exact solution of (2.3) is achieved in a number of iterations proportional to $n_t/m$ [8,12]. Assume fine-grid time stepper $\Phi$ and coarse-grid time stepper $\Psi$ are simultane-
convergence? With periodic boundary conditions, as described in the parallel-in-time solution of hyperbolic PDEs, occur in the simple setting. Consider only convergence estimates (3.1) since many of the fundamental difficulties are a special case [28]. Despite these more powerful convergence theories, in this paper, we and a more-general convergence framework developed of which these bounds represent. The fine-grid error associated with spatial mode occurs in the DFT. The eigenvalues of Φ should also satisfy |λ_k| ≤ 1 \forall k, so that the fine-grid discretization is stable. Typically this condition is also supplemented with the restriction |λ_k| < 1 \forall k; however, this is not necessary to derive the first of the following bounds nor to obtain a convergent solver. Next, let T_Δ denote the coarse-grid error-propagation matrix (that arises from considering the error propagation at only the coarse-grid points). Furthermore, let T_{Δ,k} denote the coarse-grid iteration matrix associated with the kth spatial mode, then [7, Theorem 3.3]

\[
\|T_{Δ,k}\|_2 \leq \begin{cases} 
|λ_m^k - μ_k| \sum_{j=0}^{n_t/m-1} |μ_k|^j & \text{for } \|T\|_2 \leq \sqrt{m}||T_{Δ,k}\|_2, \text{ and the fine-grid error propagation norm is } ||T||_2 = \max_k ||T_k||_2. \text{ It has been shown that these bounds are tight with respect to } n_t\text{: They are equal to } ||T_{Δ,k}||_2 \text{ up to terms of } O(m/n_t)^2 \text{ [28]. Note that the second form of the bounds in (3.1) (those on the right) holds only for } |μ_k| \neq 1. \end{cases}
\]

where the top and bottom equations apply to F- and FCF-relaxation, respectively. The fine-grid error associated with spatial mode k can be bounded by that on the coarse grid [18, Lemma 4.1], ||T_k||_2 ≤ √m||T_{Δ,k}\|_2, and the fine-grid error propagation norm is ||T||_2 = \max_k ||T_k||_2. It has been shown that these bounds are tight with respect to n_t: They are equal to ||T_{Δ,k}||_2 up to terms of O(m/n_t)^2 [28]. Note that the second form of the bounds in (3.1) (those on the right) holds only for |μ_k| \neq 1.

More recently, the analysis of [7] has been extended to the multilevel setting [18], and a more-general convergence framework developed of which these bounds represent a special case [28]. Despite these more powerful convergence theories, in this paper, we consider only convergence estimates (3.1) since many of the fundamental difficulties arising in the parallel-in-time solution of hyperbolic PDEs occur in the simple setting for which they apply. For example, in the two-level parallel-in-time solution of (2.1) with periodic boundary conditions, as described in §2.3.

Given bounds (3.1), the question is now: What is required of Ψ for fast MGRIT convergence?

1. In the case that Ψ = Φ^m, the algorithm is exact in one step; however, this is not practically feasible, since the action of Ψ should be significantly cheaper to compute than that of Φ^m. Nonetheless, (3.1) shows that convergence of a given spatial mode is related to how closely μ_k ≈ λ^m_k, and so, in general, it is necessary that the spectrum of Ψ approximate that of Φ^m in some sense.

2. From the denominators in the second form of (3.1), it is clear that modes with |μ_k| \approx 1 are potentially damped much slower than those for which |μ_k| \ll 1. This slow convergence must be rectified by ensuring the approximation μ_k \approx λ^m_k is more accurate for such modes. Given μ_k \approx λ^m_k \forall k, we have O(|μ_k|) = O(|λ_k|) when |λ_k| \approx 1. Additionally, since O(|μ_k|) = O(|λ_k|^m), we assume there is no k for which O(|μ_k|) = 1 and O(|λ_k|) \ll 1. Thus, it can be concluded that Ψ must most accurately approximate the largest (in magnitude) eigenvalues of Φ^m. As discussed in the convergence analysis of [28], the largest (in magnitude) eigenvalues of Φ, and thus those of Φ^m, typically correspond to the smoothest spatial modes. However, this is only
true in the context of dissipative spatial discretizations (like the upwind ones used here), and so it does not encompass skew-symmetric discretizations, for example. Hence, the conclusion here is equivalent to saying that \( \Psi \) must integrate spatially smooth modes similarly to \( \Phi^m \).

3. Finally, using FCF- over F-relaxation provides a mechanism for damping modes having \(|\lambda_k| < \mathcal{O}(1)\). This reinforces the notion that it is important for \( \Psi \) to best approximate the largest (in magnitude) eigenvalues of \( \Phi^m \), since error associated with modes having smaller eigenvalues can be quickly eliminated via extra relaxation, if necessary.

In summary, fast convergence necessitates the approximation \( \mu_k \approx \lambda^m_k \forall k \) hold in general, and with increased accuracy for \(|\lambda_k| \to \mathcal{O}(1)\).

3.2. Implications of convergence theory. Given the discussion above, we now provide some insight as to why convergence of MGRIT is typically much worse for advection-dominated problems compared with their diffusion-dominated counterparts. Discretizations of advection-dominated PDEs are (usually) much less dissipative than discretizations of diffusion-dominated PDEs since the PDEs themselves have only a small amount of dissipation (or none in the purely hyperbolic limit). The amount of dissipation of the \( k \)th spatial mode for a given discretization \( \Phi \) is directly related to the value of \(|\lambda_k|\). Typically, for a discretization of a diffusion-dominated problem, there are very few \(|\lambda_k| \approx 1\), with most modes satisfying \(|\lambda_k| \ll 1\), while for an accurate discretization of an advection-dominated problem, there are many \(|\lambda_k| \approx 1\). This type of behaviour can be seen in the top row of Figure 2, where the (square of the) eigenvalues of \( \Phi \) for a purely diffusive and a purely advective PDE is shown.

The fact that diffusion-dominated problems have so few \(|\lambda_k| \approx 1\) means that \( \Psi \) only has to accurately approximate very few eigenvalues of \( \Phi^m \) to yield fast convergence. Conversely, the fact that advection-dominated problems have so many \(|\lambda_k| \approx 1\), and very few \(|\lambda_k| \ll 1\), means that \( \Psi \) has to accurately approximate a much greater proportion of the eigenvalues of \( \Phi^m \). In general, this makes the task of finding a good \( \Psi \) more difficult since, by definition, we require \( \Psi \) to have simpler structure than \( \Phi^m \) so that its action is much less expensive to compute. Additionally for advection-dominated problems, eigenvalues are complex (the spatial discretization is no longer symmetric, as it often is in the pure-diffusion case) and, so, \( \Psi \) must not only approximate the magnitude of the largest eigenvalues of \( \Phi^m \), but their phases too, which has already been identified as a potential issue for 1st-order discretizations [24].

The properties just discussed, in conjunction with the plots in Figure 2, help to illuminate why rediscretization of \( \Phi \) with time step \( m \Delta t \) typically leads to a good \( \Psi \) for diffusion-dominated problems, but is often a poor choice for advection-dominated problems. As noted above, it is important for \( \Psi \) to act similarly to \( \Phi^m \) on spatially smooth modes, as these typically correspond to the largest values of \(|\mu_k|\) and \(|\lambda_k|\). This type of behaviour can be seen in Figure 2: The largest eigenvalues of \( \Phi^2 \) are clustered around spatial frequency \( \theta_k = 0 \), noting that the \( \theta_k = 0 \) eigenvalue is at position (1,0) in the top right panel. In each instance, we see that \( \mu_k \) provides a good approximation to \( \lambda^2_k \) for the smoothest modes, \( \theta_k \approx 0 \). For the diffusion problem, this approximation is adequate to obtain fast convergence as the decay of \(|\lambda_k|^2\) away from \( \theta_k = 0 \) is very rapid. However, for the advection problem, the approximation is inadequate since the decay of \(|\lambda_k|^2\) away from \( \theta_k = 0 \) is more gradual and, so, the mismatch between \( \lambda^2_k \) and \( \mu_k \) is more significant. The error propagation bounds (3.1) are shown in Figure 2 underneath the eigenvalue plots for each problem. In the diffusion case, the bound is very small and, so, convergence is fast while, in the
advection case, the bound exceeds one, indicating that the solver will be divergent. It is the smooth modes that are not accurately captured by $\Psi$ that cause the most issue. Note that the reason that $\Phi^2$ and $\Psi$ act similarly on the smoothest modes $\theta_k \approx 0$ in the first instance is because they are both consistent coarse-grid discretizations of the underlying PDEs. In the case of the periodic boundary conditions used here, this means that they both exactly capture the $\theta_k = 0$ (or constant) mode, as it is a solution of the underlying PDEs.

In summary, rediscretization provides a good approximation for the smoothest modes for a given PDE since it, along with $\Phi^m$, is a consistent coarse-grid discretization. For a diffusion-dominated problem, this approximation is adequate because even near-constant modes decay rapidly on the coarse grid under $\Phi^m$. For a typical advection-dominated discretization, however, near-constant modes decay much more slowly under $\Phi^m$, and the fact that this decay is not accurately approximated by rediscretization is detrimental to the convergence of the solver. The reason that using an alternative coarse-grid discretization (i.e., one other than rediscretization) also seldom results in a good solver for advection-dominated problems can be understood by this same line of reasoning. It should be noted that other discretizations for the PDEs shown in Figure 2 may have a different eigenvalue structure, but similar effects would be observed. A further challenge facing the parallel-in-time solution of advection-dominated problems is that explicit temporal discretizations are often used because the PDEs are not stiff, and, unlike implicit discretizations, they suffer from a CFL limit, which can complicate even further the task of identifying suitable

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**Fig. 2.** Left column: Diffusion equation $u_t = u_{xx}$ discretized with SDIRK2 in time and 2nd-order central finite-differences in space. Right column: Advection equation $u_t + u_x = 0$ discretized with SDIRK3+U3. Top row: Eigenvalues $\lambda_k^2$ of $\Phi^2$, and $\mu_k$ of $\Psi$, with $\Psi$ defined by rediscretizing $\Phi$ on an $m = 2$ temporally coarsened mesh. Bottom row: Error bound (3.1) using FCF-relaxation for each problem as a function of Fourier frequency, $\theta_k$. Both problems are subject to periodic boundary conditions in space, and are discretized on a space-time mesh covering $(x, t) \in (-1, 1) \times [0, 8]$ having $\Delta t = \Delta x = 1/64$, so that $\Phi, \Psi \in \mathbb{R}^{128 \times 128}$. 

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coarse-grid operators (see §2.3).

4. Coarse-grid operators based on a linear approximation of $\Psi_{\text{ideal}}$.

From the discussion surrounding error estimates (3.1), the coarse-grid operator $\Psi$ should somehow approximately minimize the difference between its spectrum and that of $\Phi^m$, in general, and particularly for larger $|\lambda_k|$. To this end, we consider $\Psi$ as the solution of the minimization problem

$$
\Psi := \arg \min_{\hat{\Psi} \in \mathbb{R}^{nx \times nx}} \left\| W^{1/2} |\lambda| \left[ \lambda^m - \mu(\hat{\Psi}) \right] \right\|_2^2,
$$

where $\lambda = (\lambda_1, \ldots, \lambda_{nx})^T$, $\mu = (\mu_1, \ldots, \mu_{nx})^T \in \mathbb{R}^{nx}$, and $(\lambda^m)_k \equiv \lambda^m_k$. Here, $W := \text{diag}(w) \in \mathbb{R}^{nx \times nx}$ is a weighting matrix, whose $k$th entry is $w_k := w(|\lambda_k|)$, in which $w: \mathbb{R}_+ \rightarrow \mathbb{R}_+$ is a weighting function reflecting the heuristic that it is most important to minimize $\lambda^m_k - \mu_k$ for $|\lambda_k| \rightarrow O(1)$, and less important for $|\lambda_k| \ll O(1)$. One choice of weighting function that we have found to yield relatively good results is

$$
w(z) = \frac{1}{(1 - z + \epsilon)^2},
$$

with $0 < \epsilon \ll 1$ a constant to avoid division by zero; we take $\epsilon = 10^{-6}$ in the numerical results shown here. Note that allowing a free choice for $\hat{\Psi}$ would naturally result in the choice $\Psi = \Phi^m$ and, so, the optimization in (4.1) is constrained by a pre-specified sparsity pattern of $\Psi$.

In general, the eigenvalues of a normal matrix $\Psi$ will depend nonlinearly (and non-smoothly) on its entries; that is, $\mu(\Psi)$ is a nonlinear mapping of $\Psi$, and hence, (4.1) constitutes a nonlinear minimization problem. For explicit temporal discretizations of model problem (2.1) with periodic boundaries, it is reasonable to impose that $\Psi$ is a sparse circulant matrix because $\Phi$ is and, hence, so is $\Phi^m$ (Corollary 2.2). In this section, we will also show that a sparse $\Psi$ can be used with implicit temporal discretizations of (2.1), for which $\Phi^m$ is a rational function (i.e., a dense matrix). Circulant matrices have many nice properties, one being that their eigenvalues depend only linearly on their entries (they are given by the DFT—a linear operator—applied to their first column) and, so, for this special case, (4.1) simplifies to a weighted linear least squares problem. We consider the solution of this special case throughout the reminder of this section.

Our numerical tests are limited to using FCF-relaxation, noting that the justification for using (4.1) is stronger for FCF-relaxation (see §3.1). Additionally, see Supplementary Material SM3 for the formulation and solution of a nonlinear optimization problem that is based on a more direct minimization of error estimates (3.1) than the heuristic-based minimization problem considered in this section. This more elaborate approach gives similar results.

4.1. Linear least squares formulation. Let $\hat{\Phi}^m, \hat{\psi} \in \mathbb{R}^{nx}$ denote the first columns of the circulant matrices $\Phi^m$ and $\Psi$, respectively, and note that a circulant matrix can be fully specified by its first column. Assuming the sparsity pattern of $\Psi$ is given, we let $R \in \mathbb{R}^{\nu \times nx}$ be the restriction operator that selects these $\nu$ non-zero entries from $\hat{\psi}$, where $\nu \ll nx$ since the column is sparse. The vector of unknowns is $\psi := R\hat{\psi} \in \mathbb{R}^{\nu}$, which gives the non-zero components of $\hat{\psi}$. Finally, let $F \in \mathbb{C}^{nx \times nx}$ be the DFT matrix, then due to the properties of circulant matrices, $\lambda^m = F\hat{\phi}^m$,
and \( \mu = \mathcal{F} \tilde{\psi} = \mathcal{F} R^\top \psi \). Thus, (4.1) can be written as a linear least squares problem for the non-zeros in the first column of \( \Psi \):

\[
\psi := \arg \min_{\psi \in \mathbb{R}^n} \left\| W^{1/2} \mathcal{F} \left( \hat{\phi}^m - R^\top \hat{\psi} \right) \right\|_2^2.
\]

**Remark 4.1** (\( \Psi \) minimizing \( \| \Phi^m - \Psi \|_2^2 \) is insufficient). For weighting function \( w = 1 \), or \( W = I \), (4.3) corresponds to minimizing the difference between the spectra of \( \Phi^m \) and \( \Psi \) in the two-norm. This is equivalent to minimizing the difference between \( \Phi^m \) and \( \Psi \) in the two-norm since they are both diagonalized by the same unitary transform. In this instance, the solution of (4.3) can be computed explicitly as \( \psi = R \hat{\phi}^m \), which means that \( \Psi \) is given by truncating \( \Phi^m \) in the sparsity pattern of \( \Psi \). Unsurprisingly, we have found that this choice of \( \Psi \) typically does not lead to a fast or scalable solver for model problem (2.1) because it does not adequately capture the dominant eigenvalues of \( \Phi^m \) (see §3). However, for certain problems involving ERK4+U4 and ERK5+U5 it does yield relatively good results (see Section SM3.2).

**Lemma 4.2.** The solution of (4.3) is real valued.

**Proof.** The normal equations of (4.3) are

\[
(\mathcal{F}^* W R^\top) \psi = (\mathcal{F}^* W R^\top) \tilde{\phi}^m.
\]

Since \( R \) and \( \tilde{\phi}^m \) are real, \( \psi \) is real if the circulant matrix \( A := \mathcal{F}^* W \mathcal{F} \), having eigenvalues \( w := (w_1, \ldots, w_n) \top \in \mathbb{R}^n \), is real. Letting \( \tilde{a} \) denote the 1st column of \( A \), then, because \( A \) is circulant, \( \tilde{a} = \mathcal{F}^* w \); that is, \( \tilde{a} \) is the inverse DFT of \( w \). Appealing to properties of the inverse DFT, since \( w \) is real, \( \tilde{a} \) will be real if \( w \) has even symmetry, meaning that \( w_k = w_{n-k} \). As eigenvalues of circulant matrices are known explicitly, it is easy to verify that eigenvalues \( \lambda_k \) of \( \Phi \) (or any other circulant matrix for that matter) must satisfy

\[
|\lambda_k|^2 = \lambda_k \lambda_k^* = \lambda_k \lambda_{-k} = \lambda_k |\lambda_{n-k}| = |\lambda_{n-k}|^2.
\]

It follows that \( w_k = w(|\lambda_k|) = w(|\lambda_{n-k}|) = w_{n-k} \) and, thus, \( A \) is real. 

In practice, the numerical solution of (4.3) is found to have some small imaginary components since \( \mathcal{F} \) is complex and the problem is ill-conditioned. We simply truncate these components from the solution, as is justified by Lemma 4.2. In some cases, the imaginary component can sometimes become large and simply truncating the imaginary components of such solutions has never been found to result in a good solver; see Table 3. This is also observed for some other choices of the weight matrix, \( W \), leading to particularly ill-conditioned matrices in (4.3). In practice, if an imaginary component larger than \( 10^{-8} \) is detected, we flag the results and do not accept the resulting \( \Psi \) as a coarse-grid operator. We note, however, that this does not happen for the sparsity patterns of \( \Psi \) that we advocate in the following sections.

**4.2. Explicit schemes: Selection of \( \Psi \)’s non-zero pattern.** Before solving (4.3), we must first consider the non-zero pattern of \( \Psi \). Thus far, the only constraint we have on the sparsity of \( \Psi \) is that it should be significantly sparser than \( \Phi^m \), so that time-stepping on the coarse grid is much less expensive than on the fine grid. A potentially reasonable starting point is to enforce \( \text{nnz}(\Psi) \approx \text{nnz}(\Phi) \), since this is what results from rediscretizing the PDE on a coarse grid. A useful metric for quantifying this, and, more generally, the cost of a single iteration of a solver, is the operator complexity. For a multilevel solver, this is defined as the total amount of work done in time-stepping on every level relative to that on the finest level. Let \( \Phi_\ell \) denote the time-stepping operator on level \( 1 \leq \ell \leq L \) of a multilevel hierarchy with \( L > 1 \) levels,
meaning that \( \Phi \equiv \Phi_1 \) and \( \Psi \equiv \Phi_2 \) in the two-level notation we have been using so far. Now, assuming \( \Phi_\ell \) is a sparse operator, then the work required to time-step with it is proportional to \( \text{nnz}(\Phi_\ell)n_t m^{1-\ell} \), assuming a constant coarsening factor of \( m \) on all levels. Thus, the operator complexity is given by

\[
\text{operator complexity} := \frac{1}{\text{nnz}(\Phi_1)} \sum_{\ell=1}^L m^{1-\ell} \text{nnz}(\Phi_\ell).
\] (4.4)

A scalable solver has an operator complexity that is bounded independently of the number of levels, \( L \). In fact, if one uses ideal coarse-grid operators, \( \Phi_{\ell+1} = \Phi_m^\ell \), \( 1 < \ell \leq L \), then \( \text{nnz}(\Phi_\ell) = m^\ell \text{nnz}(\Phi_1) \), and the solver has an operator complexity of \( L \), which grows like \( \log_m n_t \). In contrast, a two-level solver using our above heuristic that \( \text{nnz}(\Phi_2) \approx \text{nnz}(\Phi_1) \) has an operator complexity of roughly \( 1 + 1/m \), and a multilevel solver obeying this heuristic on all levels has a complexity bounded above by \( m/(m-1) > 1+1/m \). In the following sections, we will compare measured operator complexities with these ideal complexities.

Next, we must decide on the locations of the non-zeros themselves. Rediscretizing \( \Phi \) on a temporally coarsened mesh leads to \( \Psi \) having the same non-zero pattern as \( \Phi \); however, rediscretization does not lead to a good parallel-in-time solver for hyperbolic problems (see \S 2.3), potentially suggesting that the underlying sparsity pattern is not a good one. To motivate a better choice of sparsity pattern, we consider the effects of temporal coarsening on the exact (continuous) solution of (2.1) when it is sampled on a space-time mesh; a schematic diagram of this example is shown in Figure 3. The solution of a hyperbolic PDE is propagated through space-time along its characteristics, \( x(t) \). Advection problem (2.1) simply has characteristics that are straight lines with slope \( dx/dt = \alpha \). Now, say we have an exact fine-grid time-stepping operator, \( \Phi_{\text{exact}} \), that advects the PDE solution along characteristics from one time level to the next. (ERK1+U1 at unit CFL number corresponds to such a \( \Phi_{\text{exact}} \).) From the diagram, it is clear that \( \Phi_{\text{exact}} \) propagates the solution not only a distance of \( \Delta t \) in time, but also a distance of \( \Delta x \) in space. Considering semi-coarsening in time, by a factor of \( m = 4 \), for example, the resulting exact coarse-grid time-stepping operator is \( \Psi_{\text{exact}} = \Phi_4^{\text{exact}} \). By definition, \( \Psi_{\text{exact}} \) propagates the solution forward in time by a distance of \( 4\Delta t \); however, we see that it also propagates the solution a distance of \( 4\Delta x \) in space. Thus, coarsening in the time direction, but not in space, has shifted the spatial stencil of \( \Psi_{\text{exact}} \) (which reaches back four points in space) with respect to that of \( \Phi_{\text{exact}} \) (which reaches back one point in space). On a fundamental level, this spatial shift has occurred because, from the perspective of the PDE solution, space and time are intrinsically coupled by the characteristics. Thus, the solution operator cannot be altered with respect to one of these coordinates independently of the other.

In practice, most discretizations, like those considered in this paper, do not evolve the discrete solution precisely along the characteristics of the underlying PDE. However, they do approximate the space-time anisotropy of the PDE through non-symmetric spatial and temporal discretizations (which often use upwinding). The best non-zero pattern for \( \Psi \) for a given hyperbolic PDE will be a function of the fine-grid discretization, the coarsening factor, and the local CFL number. We wish to emphasize that appealing to the characteristics of the underlying PDE to select the non-zero pattern of \( \Psi \) will not, in general, be sufficient. Instead, one needs to consider the fine-grid discretization itself, since it is the solution to this—and not the PDE—that the coarse grid needs to accelerate. Since rediscretization does not take
into account any shift in the spatial stencil, we argue that, in general, it cannot lead to a good coarse-grid time-stepping operator for hyperbolic problems.

Given the discussion above, we now consider the selection of the non-zero pattern of $\Psi$ for ERK+U discretizations of (2.1). From an algebraic perspective and as motivated above, it is reasonable to consider a sparser spectrally equivalent approximation to $\Phi^m$ that has its sparsity pattern based on the largest non-zeros of $\Phi^m$. So to begin, we compute $\Phi^m$ and examine its non-zeros as a function of their diagonal index $i$, recalling that $\Phi^m$’s entries are constant along its diagonals since it is circulant. For $m \in \{16, 64\}$, these results are shown in Figure 4, where entries with magnitude less than $10^{-3}$ have been excluded. There is clearly a well-defined distribution in the magnitude of these non-zeros for each scheme, and they are all offset from one another, particularly for larger $m$. To explain the origin of this behaviour, we again consider the exact solution of (2.1) sampled on a space-time mesh. In a time of $m\Delta t$, the solution will travel a distance of $am\Delta t = mc\Delta x$ in space, on a grid having a CFL number (2.5) of $c$. Thus, in the context of Figure 4, where a decrement in diagonal index $i$ represents a distance of $-\Delta x$, the exact coarse-grid time-stepping operator, $\Psi_{\text{exact}}$, is represented by a value of unity at $i = -mc$. In the plots, dashed lines representing this distance for each discretization are included. Another way to interpret $mc\Delta x$ is that the characteristic arriving at $(x_i, t^{n+1})$ departed from $(x_i - mc\Delta x, t^n)$. It is clear that the clustering of the largest non-zeros for each scheme is around the characteristic departure point, $x_i - mc\Delta x$. Recall that schemes with different order have a different $c = 0.85c_{\text{max}}$ because their $c_{\text{max}}$ differ (see Table 1). Note that the peak for ERK2+U has a relatively large shift from the departure point, which is consistent with the fact that it is a fairly dispersive discretization. This illustrates, not unexpectedly, that the discretizations provide some approximation to the transportation of the solution along characteristics that occurs at the continuous level of the PDE.

From our previous intuitive arguments involving Figure 3, it is clear that the non-zero pattern of $\Psi$ should reflect the characteristic nature of the PDE; this is also the conclusion reached from an algebraic perspective of approximating $\Phi^m$ (Figure 4). We note that in [13], it was also argued that making use of characteristic information may be important. The specific sparsity patterns used for the ERK+U schemes will be discussed further in §4.3.
Fig. 4. Magnitude of diagonal entries of $\Psi_{\text{ideal}} := \Phi^m$, $m \in \{16, 64\}$, that are larger than $10^{-3}$, as a function of their diagonal index, $i$. Fine-level discretizations, $\Phi$, are ERK$p + U_p$, $p \in \{1, 2, 3, 4, 5\}$. Dashed vertical lines for each discretization are included to represent a distance of $-mc\Delta x$ from $i = 0$ (they have been excluded for $m = 1$ to reduce clutter). Note that $c = 0.85c_{\text{max}}$ is different for each scheme.

4.2.1. Note on spatial coarsening and characteristic curves. Using spatial coarsening in the parallel-in-time solution of explicit discretizations of hyperbolic PDEs seems like an attractive option since it is a natural way of overcoming coarse-grid CFL instabilities arising from coarsening only in the temporal direction. In [21], it was shown that spatial coarsening should not be applied in regions of the space-time domain where the local CFL number is small, but that even when this heuristic is obeyed, MGRIT solvers are not scalable and have large iteration counts. We now give a characteristics-based argument that spatial coarsening should not be used in MGRIT integration of hyperbolic PDEs, in general.

The solution of a hyperbolic PDE propagates along its characteristics, with the solution on a given characteristic being independent of its neighbours'. For this reason, the error associated with a given space-time approximation of the solution propagates along characteristics, and, thus, an efficient solver can only remove errors efficiently along characteristic directions. The issue concerning coarsening in space and time is that some characteristics may not be represented on the coarse grid (they simply ‘drop out’), unlike when coarsening only in time. To understand this, consider Figure 3, and imagine characteristics emanating not only from $x_{i-4}$ at time $t^n$, but all other mesh points, $x_{i-3}, x_{i-2}, x_{i-1}, x_i$, and imagine the mesh being extended rightward so that these characteristics all meet their arrival points at $t^{n+4}$. Now, if one coarsens by a factor of four in both space and time, so that $x_{i-4}$ and $x_i$ are the only spatial points retained on the coarse grid, then the characteristics departing from the points $x_{i-3}, x_{i-2}, x_{i-1}$ simply are not represented on the coarse grid. Conversely, if one coarsens only in time, all characteristics are represented on the coarse grid since their departure and arrival points are retained.

If some characteristics are not represented on the coarse grid, then the approximation along them cannot be directly corrected via a coarse-grid correction, but instead needs to be interpolated from the characteristics of their neighbours that are represented on the coarse grid. However, if the error between such characteristics truly is independent, then the interpolated coarse-grid correction will be ineffective at removing error on the characteristic being interpolated to. Consequently, the only mechanism for removing errors along such characteristics is the relaxation process on
the fine grid, but, because this is a local process, it is too slow to lead to a scalable solver. It is for this reason that spatial coarsening should not be used in MGRIT integration of hyperbolic PDEs.

Finally, we remark that the multigrid-in-time-only solution of time-dependent hyperbolic PDEs should, in some sense, be easier than the spatial multigrid solution of steady-state hyperbolic PDEs, which itself is known to be very difficult [31]. The fact that there exists a relatively simple direction (time) for the former in which information consistently flows is a significant advantage because it naturally lends itself to coarsening since all characteristics cross lines of constant \( t \). For the case of steady-state hyperbolic PDEs, however, if one wishes to represent fine-scale characteristics on the coarse-grid (as we have argued above is necessary for an efficient multilevel solution of a hyperbolic PDE), then, in general, one must coarsen along characteristics themselves which is by no means trivial when characteristics may curve in any direction and may even close upon themselves.

4.3. Explicit schemes: Two-level results. In this section, we show MGRIT convergence when solving least squares problem (4.3) for ERK discretizations with varying coarsening factors. To demonstrate the validity of the ideas outlined in the previous section, we solve the least squares problem for \( \Psi \) having a sparsity pattern equal to that of the fine-level operator \( \Phi \), and for it having a sparsity pattern inspired by \( \Phi^m \).

The solver iteration counts for \( \Psi \) having the same sparsity pattern as \( \Phi \) are shown in the left side of Table 3. A convergent solver was not obtained for any \( m \) for the 1st-order scheme, convergent schemes were obtained only for \( m = 2 \) for the 2nd- and 3rd-order schemes, and convergent schemes with \( m \in \{2, 4, 8\} \) were obtained for the 4th- and 5th-order schemes. In all cases where convergent solvers were found, the iteration counts remain constant as the mesh is refined. For the cases where the solvers converge, these results are certainly an improvement on those using rediscretization, which are divergent in this setting due to coarse-level CFL instability (see §2.3), attesting to the power of the optimization approach. However, for many coarsening factors and discretizations, the results are significantly worse than those obtained when using a sparsity pattern based on \( \Phi^m \), as shown in the right side of Table 3. Indeed, a reasonable heuristic seems to be that when there is a large overlap between the location of non-zeros of \( \Phi \) and the largest non-zeros in \( \Phi^m \), fast and scalable solvers were found for \( \Phi \) and \( \Psi \) sharing a non-zero pattern.

Keeping in mind that our main goal in this paper is to demonstrate that there exist coarse-grid time-stepping operators for MGRIT that lead to very fast and scalable convergence for linear advection in just a handful iterations as shown in Table 3, we now explain in detail how the sparsity patterns were chosen that lead to the results in the right-hand side of Table 3, and then give a general discussion about the solvers. To select this sparsity pattern for a given discretization and coarsening factor, we first look at the locations of the largest non-zeros in \( \Psi_{\text{ideal}} \) (as in Figure 4). As a first approximation, we choose a contiguous subset of the locations of the largest \( \text{nnz}(\Phi) \) non-zeros of \( \Phi^m \), where \( \text{nnz}(\Phi) \) denotes the number of non-zeros in each row of \( \Phi \) (even if the locations of the largest non-zeros are not contiguous). A set of test problems is then run to determine if a scalable solver results. If it does not, then an extra non-zero is included in a contiguous fashion and the experiments are re-run; this process is repeated until a scalable solver is obtained.

Additionally, once a scalable solver has been found, if it is determined that the convergence is significantly improved by including a relatively small number of ad-
Two-level iteration counts for ERK+U discretizations with $\Psi$ as linear least squares solution (4.3). Left: Sparsity pattern of $\Psi$ is equal to that of $\Phi$. Right: Sparsity pattern of $\Psi$ is based on that of $\Phi^m$. An ‘*’ denotes a solve that did not converge to the required tolerance in significantly fewer than $n_t/(2^m)$ iterations (i.e., the number of iterations at which the exact solution is reached); an ‘x’ denotes a solve in which the least squares solution had imaginary components larger than $10^{-8}$, as another indication of divergence.

| Scheme | $n_x \times n_t$ | $m$ (Φ-based sparsity) | $m$ ($\Phi^m$-based sparsity) |
|--------|------------------|-------------------------|-----------------------------|
|        |                  | 2 4 8 16 32 64          | 2 4 8 16 32 64               |
| ERK1+U1| $2^8 \times 2^{10}$ | x x x x x x x           | 11 6 6 7 6 5                |
|        | $2^{10} \times 2^{12}$ | x x x x x x x x x       | 11 6 6 7 6 5                |
|        | $2^{12} \times 2^{14}$ | x x x x x x x x x x     | 11 6 6 7 6 5                |
| ERK2+U2| $2^8 \times 2^{11}$ | x x x x x x x x         | 10 7 9 8 7 7                |
|        | $2^{10} \times 2^{13}$ | x x x x x x x x x       | 10 7 9 8 7 7                |
|        | $2^{12} \times 2^{15}$ | x x x x x x x x x x     | 10 7 9 8 7 7                |
| ERK3+U3| $2^8 \times 2^9$ | x x x x x x x x         | 7 6 5 6 5 3                 |
|        | $2^{10} \times 2^{11}$ | x x x x x x x x x x     | 7 6 5 6 5 4                 |
|        | $2^{12} \times 2^{13}$ | x x x x x x x x x x x   | 7 6 5 6 5 4                 |
| ERK4+U4| $2^8 \times 2^{10}$ | x x x x x x x           | 5 4 4 4 5 5                 |
|        | $2^{10} \times 2^{12}$ | x x x x x x x x x       | 5 4 4 4 5 6                 |
|        | $2^{12} \times 2^{14}$ | x x x x x x x x x x     | 5 4 4 4 5 6                 |
| ERK5+U5| $2^8 \times 2^9$ | x x x x x x x           | 3 3 3 4 4 3                 |
|        | $2^{10} \times 2^{11}$ | x x x x x x x x x x     | 3 3 3 4 4 4                 |
|        | $2^{12} \times 2^{13}$ | x x x x x x x x x x x   | 3 3 3 4 4 4                 |

Note: Additional non-zeros (e.g., two or three), then that is done also. However, there has been no serious attempt to optimize the convergence rate as a function of the number of non-zeros. As an example, the left panel of Figure 5 shows the non-zero patterns of $\Psi$ selected for ERK3+U3 as a function of coarsening factor, $m$. Figure 5 also shows (right panel), for each discretization, the operator complexities (4.4) of the resulting solvers along with the operator complexity of $1+1/m$ that results when $\text{nnz}(\Psi) = \text{nnz}(\Phi)$ in a two-level method (see §4.2).

We find that, in general, to obtain convergent and scalable solvers there has to be a slight increase in the number of non-zeros in $\Psi$ as the coarsening factor is increased, as can be seen for ERK3+U3 in Figure 5 (left panel), for example. The number of additional non-zeros required is smaller for higher-order discretizations, which is likely a consequence of their smaller levels of dissipation. This behaviour can be seen in the right panel of Figure 5, where operator complexities for a given $m$ tend to be small for higher-order methods. Also notice that ERK4+U4 and ERK5+U5 essentially have operator complexities of $1+1/m$ which is reflective of the fact that very few if any additional non-zeros were needed in $\Psi$. Nonetheless, Figure 5 shows that the increasing number of non-zeros in $\Psi$ with $m$ for the lower-order schemes is acceptable since the operator complexity continues to decrease.

The results at the right of Table 3 convincingly show that it is possible to overcome the CFL instability that arises from rediscretizing the fine-grid discretization on a temporally coarsened mesh and to obtain very fast multigrid convergence, and therefore show the significance of using a characteristic-inspired sparsity pattern for $\Psi$. Notably, the convergence rates of the solvers shown in Table 3 are comparable, and in some instances much faster, than for model diffusion problems using redis-
cretized coarse-grid operators [7, 8]. To the best of our knowledge, these are the first scalable results obtained with a two-level time-coarsening algorithm for the explicit discretization of any hyperbolic PDE using realistic CFL numbers, and also for moderately-large coarsening factors. As discussed above, standard approaches for this problem are mostly either divergent or not scalable, with iteration counts much larger than those presented here [20, 21]. Interestingly, convergence rates tend to be faster for higher-order discretizations compared with those of lower order. When combined with the trend in Figure 5 (right panel) that operator complexities are smaller for higher-order discretizations, this suggests that higher-order discretizations of model problem (2.1) likely benefit more from parallel-in-time integration. Overall, these results indicate that if suitable coarse-grid operators are used, the parallel-in-time solution of hyperbolic PDEs with MGRIT may have the potential to be as successful as it has been for diffusion-dominated problems. This is investigated further in §5 through parallel studies.

Finally, an example of the eigenvalues and entries of \( \Psi \) for ERK3+U3 with \( m = 8 \) is shown in Figure 6. In this example, the eigenvalues of \( \Phi^8 \) are clearly very well approximated by the eigenvalues of \( \Psi \) when they are of order one (in magnitude), and not so well approximated when they are smaller. Given this behaviour, it is unsurprising that the solver converges quickly, and that the associated error bounds are small (bottom right of the figure). The entries of the least squares \( \Psi \) (upper right panel of Figure 6) are clearly correlated with those of the ideal operator.

Remark 4.3 (Mesh-independence of least squares solution (4.3)). For a given discretization and coarsening factor, we numerically observe that the error in the least squares solution (4.3) converges to a constant as \( n_x \to \infty \). This feature of the least squares solution is perhaps unsurprising given the entries of \( \Psi_{\text{ideal}} \) are also independent of the mesh resolution: \( \Delta x \) and \( \Delta t \) appear in \( \Theta \) only in the form of the CFL number (2.5) and, so, if the mesh is refined such that the CFL number is kept constant (as it is here), then the entries in \( \Psi_{\text{ideal}} := \Phi^m \) are constant with respect to \( \Delta x \) and \( \Delta t \).

Remark 4.4 (Similarity of \( \Psi \) and semi-Lagrangian discretizations). While the construction of the coarse-grid operators here is purely algebraic, based on optimization
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Problem (4.3), it would be pleasing if they were related or similar to a consistent discretization of the underlying PDE. The non-local stencil structure prohibits a relationship with a standard type of discretization, but it is related with the form of an explicit semi-Lagrangian discretization. However, given that we have to increase the size of the stencil with the coarsening factor to get a scalable solver (see Figure 5), the coarse-grid operators are clearly not just a specific semi-Lagrangian discretization of the PDE on coarsened grids. This is consistent with the results of [26], where fast convergence was not obtained for their model hyperbolic problem when employing a semi-Lagrangian coarse-grid operator. Nonetheless, this is a promising area to consider for future research.

An application of ideas analogous to those in this section but to discretizations of (2.1) with inflow/outflow boundary conditions—rather than periodic ones—can be found in Supplementary Material SM2.

4.4. Explicit schemes: Multilevel results. In this section, we develop near-optimal coarse-grid operators for multilevel solvers. The scalability of the two-level solvers considered in the previous section is limited because they require the sequential solve of a large coarse-grid problem. Of course, large coarsening factors can be employed to reduce the bottleneck presented by sequential coarse-grid solves, but developing good coarse-grid operators for large coarsening factors presents additional difficulties. Conversely, multilevel solvers are more scalable because the temporal grid can be coarsened gradually over many levels until the coarsest level contains sufficiently few degrees of freedom that a sequential solve there does not present a significant bottleneck.

Convergence theory of multilevel MGRIT is significantly more complicated than in the two-level setting [18] and, so, rather than approximately minimizing a multilevel convergence estimate as we did in the two-level case, we simply consider applying our previous two-level strategy in a recursive fashion. That is, if level \( \ell \) uses a time-

Fig. 6. Weighted linear least squares solution (4.3) for ERK3+U3 with \( n_x \times n_t = 2^8 \times 2^9 \), coarsening factor \( m = 8 \), and the sparsity pattern of \( \Psi \) based on that of \( \Phi \). Left: Eigenvalues \( \mu_{\text{ideal}} := \lambda^8 \) of ideal coarse-grid operator \( \Psi_{\text{ideal}} := \Phi^8 \), and those of the linear least squares approximation, \( \mu_{\text{linear}} \). Top right: Entries of \( \Psi_{\text{ideal}} \) with magnitude larger than \( 10^{-3} \) as a function of their diagonal index, \( i \), and all entries in the linear least squares approximation. Bottom right: Two-level FCF-error bounds (3.1) associated with the linear least squares coarse-grid operator as a function of spatial Fourier frequency.
stepping operator $\Phi_\ell$, and coarsens by a factor of $m$, then the ideal time-stepping operator on level $\ell + 1$, $\Psi_{\text{ideal},\ell+1} := \Phi_\ell^m$, is approximated with linear least squares problem (4.3). As previously, sparsity patterns of coarse-grid operators are selected by roughly choosing some subset of the locations of the largest non-zeros in the corresponding ideal coarse-grid operator. Again, we try to strike some balance between the overall convergence rate of the solver and the amount of fill-in of the coarse-grid operators.

For the sake of brevity, we only show results for ERK$p+U_p$, $p \in \{1, 3, 5\}$ since general conclusions about ERK2+U2 and ERK4+U4 can be made based on their two-level performance relative to that of their neighbours’ tested here. We have considered both V- and F-cycles using coarsening factors of both $m = 2$ and $m = 4$. However, only results for V-cycles using $m = 4$ coarsening are shown here because we found that this combination typically resulted in the fastest parallel solvers (see §5). For the case of ERK1+U1, we coarsen down to a minimum of just four points on the coarsest grid in time, and for ERK3+U3 and ERK5+U5, we coarsen down to a minimum of just eight points on the coarsest grid in time.

The iteration counts for the resulting solvers are shown in Table 4 as a function of mesh resolution and number of grid levels. For all three discretizations, the solvers appear scalable with respect to the number of levels in the grid hierarchy and the mesh size, and they are very fast. We find that to obtain scalable solvers, the number of non-zeros in coarse-grid operators has to increase relative to that of the operator on the previous level. Similarly to the two-level case (see Figure 5), the amount of fill-in required decreases with increasing discretization order, as is reflected by the decreasing operator complexities also shown in the table. Importantly, the operator complexities converge to a constant as the number of levels is increased, which, when taken with the scalable iteration counts, indicates that the amount of work to solve a given problem is independent of the number of grid levels.

To the best of our knowledge, this is the first time that scalable multilevel results have been obtained for the explicit discretization of any hyperbolic PDE using a realistic CFL fraction. For example, [21] is the only other work to show multilevel MGRIT results (with spatial coarsening) for explicit discretizations of hyperbolic problems, yet results presented there were limited to first-order accuracy, used a smaller CFL fraction, and even with the use of F-cycles, were not scalable with respect to mesh size. Furthermore, convergence was slow, with on the order of 40 iterations required to reach convergence for the mesh sizes considered here.

4.5. Implicit schemes. We now consider linear least squares problem (4.3) for the computation of near-optimal coarse-grid operators $\Psi$ for SDIRK+U discretizations of (2.1). As discussed in §2, for such discretizations, $\Phi$ is a rational function of sparse matrices and so, too, is $\Psi_{\text{ideal}} := \Phi^m$. Naturally, one might seek a $\Psi$ that is also of this form. However, it is not obvious how this should be done, with one complication being the choice of sparsity patterns for the numerator and denominator. Consequently, we take a different approach here.

Since $\Phi$ is a rational function of sparse matrices, it can also be written as a dense matrix. To assess to what extent $\Phi$ and $\Phi^m$ do globally couple the solution, we form them as dense matrices and consider the magnitude of their entries as a function of their diagonal index, as pictured in Figure 7 for $m \in \{16, 64\}$, where entries with magnitude smaller than $10^{-3}$ have been truncated. These plots show that, despite $\Phi$ and $\Phi^m$ being dense matrices, they effectively act as sparse matrices, with their largest non-zeros having a sharp peak that is correlated with the characteristic departure
Table 4  
Multilevel iteration counts as a function of number of grid levels for V-cycles using FCF-relaxation with \( m = 4 \) coarsening on each level. Operator complexities (OC) (4.4) are also given for each discretization. Note the ideal operator complexity for a multilevel method is bounded above by \( m/(m−1) = 1.33 \ldots \) for \( m = 4 \) (see §4.2). A ‘-’ denotes a hierarchy that would have coarsened to fewer than the prescribed minimum number of allowable points (four for ERK1+U1, and eight for ERK3+U3 and ERK5+U5).

| Scheme           | \( n_x \times n_t \) | Number of levels |               |               |               |               |               |
|------------------|-----------------------|------------------|---------------|---------------|---------------|---------------|---------------|
|                  |                       | 2               | 3             | 4             | 5             | 6             | 7             |
| ERK1+U1          | \( 2^8 \times 2^{10} \) | 6               | 6             | 6             | -             | -             | -             |
|                  | \( 2^{10} \times 2^{12} \) | 6               | 7             | 7             | 7             | -             | -             |
|                  | \( 2^{12} \times 2^{14} \) | 6               | 7             | 7             | 7             | 7             | -             |
|                  | OC                    | 1.38            | 1.56          | 1.65          | 1.69          | 1.71          | 1.71          |
| ERK3+U3          | \( 2^8 \times 2^9 \)  | 6               | 7             | 7             | -             | -             | -             |
|                  | \( 2^{10} \times 2^{11} \) | 6               | 7             | 7             | 7             | -             | -             |
|                  | \( 2^{12} \times 2^{13} \) | 6               | 7             | 7             | 8             | 8             | -             |
|                  | OC                    | 1.28            | 1.35          | 1.38          | 1.38          | 1.39          | -             |
| ERK5+U5          | \( 2^8 \times 2^9 \)  | 3               | 4             | 4             | -             | -             | -             |
|                  | \( 2^{10} \times 2^{11} \) | 3               | 4             | 5             | 5             | -             | -             |
|                  | \( 2^{12} \times 2^{13} \) | 3               | 4             | 5             | 5             | 5             | -             |
|                  | OC                    | 1.25            | 1.31          | 1.33          | 1.33          | 1.33          | -             |

The effectively sparse structure of \( \Psi_{\text{ideal}} \)—as shown in Figure 7—begs the question: Can a sparse/explicit coarse-grid operator \( \Psi \) be used to approximate it? The use

Fig. 7. Magnitude of diagonal entries of the dense matrices \( \Psi_{\text{ideal}} := \Phi^m, m \in \{16, 64\} \), that are larger than \( 10^{-3} \), as a function of their diagonal index, \( i \). Fine-level discretizations, \( \Phi \), are SDIRKp+U_p, \( p \in \{1, 2, 3, 4\} \). A value of \( n_x = 2^{10} \) has been used here. In each plot, a dashed vertical line is included to represent a distance of \(-4m\Delta x\) from \( i = 0 \) (these schemes use CFL number of \( c = 4 \)).
of an explicit coarse-grid operator with an implicit fine-grid discretization is certainly not standard, and in fact, the reverse case has been used elsewhere in the literature: An implicit coarse-grid operator has been coupled with an explicit fine-grid discretization since it is a natural way of ensuring that the coarse-grid operator is stable [8]. However, quasi-tracking the solution of the PDE along characteristics—as done in the previous sections—is another way of ensuring the coarse-grid operator is stable, since the physical domain of dependence is included in the numerical domain of dependence.

We now test the idea of using a sparse $\Psi$ to approximate a dense $\Phi^m$. As for the ERK discretizations, we place a restriction on the number of non-zeros in $\Psi$. To do so, we compute the entries in the 1st column of $\Phi^m$ (this can be done relatively inexpensively using the DFT and its inverse), and then we select a non-zero pattern using thresholding. That is, recalling $\tilde{\phi}^m$ is the (dense) first column of $\Phi^m$, we take the non-zero pattern to be that of the entries with magnitude at least equal to $\eta_{tol} \times \max_k |\phi^m_k|$, in which $\eta_{tol} < 1$. Unsurprisingly, we find that smaller values of $\eta_{tol}$ lead to more quickly converging MGRIT solvers. As for the ERK schemes, we have loosely tried to achieve some balance between the rate of convergence and the number of non-zeros in $\Psi$, but this has not been fully optimized. For each discretization and coarsening factor, $m$, we allow for a different value of $\eta_{tol}$. For $m \in \{2, 4, 8, 16, 32, 64\}$ the values for the $p$th-order SDIRK+U scheme are: $p = 1, \eta_{tol} = \{.1, .125, .25, .5, .6\}$; $p = 2, \eta_{tol} = \{.05, .1, .2, .5\}$; $p = 3, \eta_{tol} = \{.005, .01, .02, .04\}$; and $p = 4, \eta_{tol} = \{.005, .01, .02, .04\}$. These choices of $\eta_{tol}$ result in coarse-grid operators that have on the order of the same number of entries shown in the plots in Figure 7. Figure 8 shows the number of non-zeros per row of $\Psi$ as a function of the coarsening factor and how there is, in general, some growth in this number with $m$, just as there is in the number of non-zeros in $\Phi^m$ whose magnitude is significant (Figure 7).

![Fig. 8. Number of non-zeros per row of $\Psi$ for SDIRK+U discretizations as a function of coarsening factor, $m$.](image)

The iteration counts for the solvers are shown in Table 5. Convergence is relatively fast for all coarsening factors, and the solvers appear scalable as the mesh is refined. This is in stark contrast to the results in Table 2 where rediscretizing $\Phi$ on the coarse grid resulted in a divergent solver for all discretizations except for SDIRK1+U1. Therefore, we have shown once again that there exist significantly better coarse-grid operators for advection problem (2.1) than those offered by rediscretizing the PDE on the coarse grid. Furthermore, these results confirm that despite $\Phi^m$ being a dense operator for the implicit temporal discretizations considered here, it can be
well approximated by a sparse one.

Table 5
Two-level iteration counts using FCF-relaxation for SDIRK+U discretizations with $\Psi$ given as linear least squares solution (4.3).

| Scheme       | $n_x \times n_t$ | $m$ |
|--------------|------------------|-----|
| SDIRK1+U1   | $2^{10} \times 2^{10}$ | 2   |
|             | $2^{12} \times 2^{12}$ | 4   |
| SDIRK2+U2   | $2^{10} \times 2^{10}$ | 2   |
|             | $2^{12} \times 2^{12}$ | 4   |
| SDIRK3+U3   | $2^{10} \times 2^{10}$ | 2   |
|             | $2^{12} \times 2^{12}$ | 4   |
| SDIRK4+U4   | $2^{10} \times 2^{10}$ | 2   |
|             | $2^{12} \times 2^{12}$ | 4   |

5. Parallel results. In this section, we present strong parallel scaling results for the ERK$p$+U$p$, with $p \in \{1, 3, 5\}$, multilevel solvers developed in §4.4. We show that they can lead to significant speed-ups over sequential time marching. Parallel results for the two-level solvers developed in §4.3 can be found in Supplementary Material SM4.

The implementations use the open-source package XBraid [1]. The results were generated on Quartz, a Linux cluster at Lawrence Livermore National Laboratory consisting of 2,688 compute nodes, with thirty-six 2.1 GHz Intel Xeon processors per node. For each discretization, we consider the strong scaling of a single problem whose space-time grid is the largest from Table 4, and the number of levels in the solver is taken as the maximum shown in this table. Since we want to demonstrate the benefits of parallelization in time, we only consider parallelization in the time direction. As throughout the rest of this paper, we first consider a stopping criterion based on achieving a space-time residual below $10^{-10}$ in the discrete $L^2$-norm, but a stopping criterion based on achieving discretization error accuracy is also considered.

In our parallel tests, we have considered both V- and F-cycles with coarsening factors of $m = 2$ and $m = 4$. We find that F-cycles require fewer iterations to converge than V-cycles, but this of course comes at the cost of added work and communication. Accordingly, we typically find that the best results arise from the use of V-cycles with $m = 4$ coarsening and, thus, results for this configuration are shown here, in Figure 9. The plots show good parallel scaling with benefit over sequential time-stepping when using at least 32 processors in almost all cases, which is on par with what has been achieved for model diffusion-dominated problems using time-only parallelism [9]. The largest speed-up achieved over sequential time-stepping is at 1024 processors, where MGRIT is faster by a factor of about 3.8, 8.4, and 18.1 when solving up to $10^{-10}$ residual tolerance, and of about 10.0, 12.6, and 13.7 when solving up to discretization error (for the discretizations in the order of increasing accuracy).

The relative speed-ups shown here further demonstrate the improvements given by this work over existing parallel-in-time strategies for hyperbolic PDEs. For example, achieving MGRIT speed-up with high-order discretizations of any hyperbolic problem is unheard of in the literature, and so the fact that we have been able to achieve a speed-up on the order of 15 times for a highly accurate explicit 5th-order discretization run at a realistic CFL fraction is significant.
6. Conclusions. In this paper, we consider the parallel-in-time integration of the one-dimensional, constant-coefficient linear advection problem using the MGRIT and Parareal algorithms. This PDE represents the simplest of all hyperbolic problems, yet, to the best of our knowledge, no parallel-in-time solvers have been successfully applied to accurate discretizations of this problem, yielding relatively inexpensive solvers that achieve fast and scalable convergence for realistic CFL fractions close to one. We use existing convergence theory to explain why this problem is so difficult, and what is required of coarse-grid operators for its efficient solution. Convergence hinges on the coarse-grid operator accurately propagating slowly-decaying spatial modes through time very similarly to the fine-grid operator. The larger number of such modes for advection-dominated problems compared with diffusion-dominated problems means that even small differences between fine- and coarse-grid operators typically results in extremely poor convergence.

For this PDE, we develop near-optimal coarse-grid operators through the approximate minimization of error estimates. We apply these coarse-grid operators to both explicit and implicit discretizations of low- and high-order accuracy and demonstrate that they lead to solvers with fast and scalable convergence that is on par with performance typically seen from these parallel-in-time algorithms when applied to diffusion-dominated problems. For explicit discretizations, we show that it is possible to overcome the CFL-driven divergence that arises from naively applying a conditionally stable discretization on the coarse grid. Primarily, this is done by tracking information along characteristic curves of the PDE on the coarse grid. Moreover, we show that observing this characteristic nature is also important for unconditionally stable implicit discretizations. Finally, our results indicate that higher-order discretizations of this problem benefit more from parallel-in-time integration compared with those of lower-order.

The coarse-grid operator selection techniques developed here are very powerful, allowing us to demonstrate that scalable and very fast solvers are possible when coarse-grid operators approximately track information flow along characteristics. This approach also shows that efficient methods are not possible when employing coarse-grid operators that use only local information (as rediscretization does). While the optimization approach is powerful, it also has clear limitations, requiring the solution of
expensive optimization problems. Further, it is not directly generalizable to PDEs more complicated than constant-coefficient linear advection. However, we expect that the heuristic insights developed here, in particular, that coarse-grid operators should track characteristic information, will be important for more complicated hyperbolic problems. Future work will focus on developing practical coarse-grid operators for linear advection as well as for more complicated hyperbolic problems which are of practical interest, such as those with non-constant coefficients and nonlinearities. Our major finding, that coarse operators need to track characteristics, will be a central guiding principle in this future work; indeed, this has already led to some promising results in initial research in these directions. Furthermore, the spatial parallelization of the coarse-grid operators developed here will also be considered, which is not straightforward due to their non-local structure in space.

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SUPPLEMENTARY MATERIALS: OPTIMIZING MGRIT AND PARAREAL COARSE-GRID OPERATORS FOR LINEAR ADVECTION∗

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SM1. Runge-Kutta Butcher tableaus. In this section, Butcher tableaus are given for the Runge-Kutta (ERK) methods used in the main text. Explicit Runge-Kutta (ERK) methods are given in Tables SM1 and SM2. L-stable singly diagonally implicit Runge-Kutta (SDIRK) methods are given in Tables SM3 and SM4.

| Table SM1 | Butcher tableaus for first-, second- and third-order ERK methods. |
|-----------|------------------------------------------------------------------|
| ERK1      | ERK2 [19, (9.7)]                                                 |
|           | [19, (9.8)]                                                     |
| 0         | 0 0 0 0                                                         |
| 0         | 1 0 0 0                                                         |
| 0         | 1 0 0 0                                                         |
| 1         | 1/2 1/2                                                         |
|           | 1/6 1/6 2/3                                                     |

SM2. Application of two-level solvers to inflow/outflow boundaries.
The techniques discussed for finding near-optimal Ψ formally apply only to discretizations of (2.1) with periodic boundary conditions, as they rely on Φ and Ψ being circulant. Inflow/outflow boundary conditions do not result in circulant Φ and, in fact, Φ may no longer even be diagonalizable, since Φ will be a non-normal matrix, unlike in the case of periodic boundaries. Thus, the convergence theory in [7] cannot be applied as it assumes Φ is unitarily diagonalizable. Hence, the rigorous optimization of Ψ for such problems would require the use of more complicated convergence theory, such as that developed in [28], and the resulting optimization problem would certainly be highly nonlinear.
Table SM2

Butcher tableaus for fourth- and fifth-order ERK methods.

| ERK4 [2, p. 180] | ERK5 [2, (236a)] |
|------------------|------------------|
| 0                | 0                |
| 1/4              | 1/4              |
| 0 0 0 0 0        | 1/4 1/8 1/8 0 0 0|
| 1/2 1/2 0 0 0    | 1/2 0 0 1/2 0 0 0|
| 1/2 0 1/2 0 0    | 3/4 3/16 -3/8 3/8 9/16 0 0|
| 1 0 0 1 0        | 1 -3/4 8/7 6 12/7 8 0|
| 1/5 1/3 1/5 1/5 1/5 | 7/90 0 32/90 12/32 32/32 7/90 |

Table SM3

Butcher tableaus for first- and second-order SDIRK methods.

| SDIRK1 | SDIRK2 [2, p. 261] |
|--------|-------------------|
| 1      | 1 - \sqrt{2} / 2 |
| 1      | 1 - \sqrt{2} / 2 |

Table SM4

Butcher tableaus for third- and fourth-order SDIRK methods. The constants used in SDIRK3 are: \( \zeta = 0.43586652150845899942 \ldots, \alpha = \frac{1 + \zeta}{2}, \beta = \frac{1 - \zeta}{2}, \gamma = -\frac{1}{2} \zeta^2 + 4 \zeta - \frac{1}{4}, \epsilon = \frac{3}{2} \zeta^2 - 5 \zeta + \frac{5}{4} \).

| SDIRK3 [2, p. 262] | SDIRK4 [32, (6.16)] |
|---------------------|---------------------|
| \zeta               | \zeta 0 0           |
| 1/4                 | 1/4 0 0 0 0        |
| 3/4                 | 1/2 1/4 0 0 0     |
| 11/20               | 17/50 -1/25 1/4 0 0|
| \alpha \beta \zeta 0 | \zeta 0       |
| 1/2                 | 371/1360 -137/2720 15/544 1/4 0|
| 1 \gamma \epsilon \zeta | 1             |
| 25/24               | 25/24 -49/48 123/16 -85/12 1/4|
| \gamma \epsilon \zeta | \zeta 0       |
| 25/24               | 25/24 -49/48 123/16 -85/12 1/4|

In the spirit of local Fourier analysis of multigrid methods [30], we hypothesise that a near-optimal \( \Psi \) designed for a problem subject to periodic boundaries may work well for a problem with inflow/outflow boundaries, since for inflow/outflow boundaries, \( \Phi \) has Toeplitz structure in the interior of the domain, but not in the vicinity of
the boundaries. To test this hypothesis, we take the near-optimal circulant \( \Psi \) for the analogous periodic problem (i.e., having the same discretization, CFL number, \( n_z \), and \( m \)), and we truncate it such that it is no longer circulant (but is still Toeplitz). This is then used as the coarse-grid operator for the inflow/outflow problem. We have also tested not truncating the operator, but this leads to slightly less satisfactory results. Given the upwind-biased non-zero pattern of the circulant coarse-grid operators from the previous section, for moderate \( m \), truncating these operators results in strictly lower triangular Toeplitz matrices.

In the numerical tests, an inflow boundary condition is prescribed at \( x = -1 \), and there is an outflow at \( x = 1 \). The inflow condition is chosen as \( u(-1,t) = \sin^4(\pi t) \), which corresponds to the continuous solution of (2.1) that is propagated off the right hand side of the domain. We choose this boundary condition as it is a simple way of ensuring continuity of derivatives across the boundary at \( t = 0 \) that are required by the spatial discretizations to achieve full accuracy there. While this choice of inflow condition leads to a solution that mimics the periodic solution (they converge to the same solution as the mesh is refined), we stress that this does not influence the convergence of MGRIT, which is independent of the solution vector for linear problems [28]. Numerical tests (not shown here) using non-periodic inflow boundary conditions also confirm this.

For the numerical implementation, sufficiently accurate extrapolation is used at the outflow boundary; at the inflow boundary, sufficiently accurate ERK stage values are computed using ideas similar to those in [3], except we elect to use the same spatial discretization right up to the boundary rather than switching to a compact one. To approximate solution and ERK stage values at ghost points, we employ truncated Taylor series about the boundary and use the PDE with the ‘inverse Lax–Wendroff’ procedure to interchange spatial derivatives for temporal derivatives of the inflow condition [19, p. 364]. For each scheme, numerical tests (not shown here) have been used to verify that convergence at the theoretically predicted rate is achieved (order \( p \) for an ERKp+Up scheme). Numerical tests also indicate that CFL limits of these schemes are very similar to their analogues with periodic boundaries (Table 1). Also note that standard rediscretized coarse-grid operators for these boundary conditions result in divergent behaviour, as for the periodic problem (see §2.3).

The iteration counts for the inflow/outflow boundary problem are given in Table SM5. For the most part, the results are indistinguishable from those for the periodic problem (Table 3). The only differences are that, at smaller resolutions, convergence is occasionally slightly faster for the inflow/outflow problem, and iteration counts of ERK5+U5 with coarsening factors \( m = 2, 4 \) have increased from the periodic problem. Thus, the near-optimal coarse-grid operators for the periodic problem also make excellent coarse-grid operators for the inflow/outflow problem despite the fact that they were not designed to do so in a rigorous sense. These results indicate that the issues hindering convergence for hyperbolic problems in the simpler periodic setting, where \( \Phi \) and \( \Psi \) are normal matrices, are also responsible for poor convergence in this more complicated setting.

**SM3. Coarse-grid operators based on a nonlinear approximation of \( \Psi_{\text{ideal}} \).** In §4, coarse-grid time-stepping operators were sought through a linear least squares procedure that used heuristics based on convergence theory (see §3.1). To better understand how accurate this heuristic-driven approach was, in this section, we formulate and solve a nonlinear optimization problem that approximately minimizes error estimates (3.1) in a more direct way. We find no significant difference between the
Two-level iteration counts using FCF-relaxation for ERK+U discretizations of model problem (2.1) with inflow/outflow boundaries; \( \Psi \) is given by truncating the circulant matrix resulting from linear least squares solution (4.3), with its sparsity pattern based on that of \( \Psi_{\text{ideal}} \).

| Scheme     | \( n_x \times n_t \) | \( m \) |
|------------|-----------------------|-------|
| ERK1+U1    | \( 2^8 \times 2^{10} \) | 2 4 8 16 32 64 |
|            | \( 2^{10} \times 2^{12} \) | 10 6 6 6 5 3 |
|            | \( 2^{12} \times 2^{14} \) | 11 6 6 7 6 5 |
| ERK2+U2    | \( 2^8 \times 2^{14} \) | 2 10 7 8 6 4 |
|            | \( 2^{10} \times 2^{13} \) | 10 7 9 8 7 7 |
|            | \( 2^{12} \times 2^{15} \) | 10 7 9 8 7 7 |
| ERK3+U3    | \( 2^8 \times 2^9 \) | 2 7 6 5 5 4 |
|            | \( 2^{10} \times 2^{11} \) | 7 6 5 6 5 4 |
|            | \( 2^{12} \times 2^{13} \) | 7 6 5 6 5 4 |
| ERK4+U4    | \( 2^8 \times 2^{10} \) | 2 5 4 4 4 3 |
|            | \( 2^{10} \times 2^{12} \) | 5 4 4 4 5 5 |
|            | \( 2^{12} \times 2^{14} \) | 5 4 4 4 5 6 |
| ERK5+U5    | \( 2^8 \times 2^9 \) | 2 8 5 4 4 2 |
|            | \( 2^{10} \times 2^{11} \) | 8 5 3 4 4 4 |
|            | \( 2^{12} \times 2^{13} \) | 7 5 3 4 4 4 |

Convergence rates of the MGRIT solvers arising from this more direct and elaborate nonlinear minimization and those of the simpler, heuristic-based, linear minimization of §4. These results indicate that the heuristics developed in §3.1 are accurate and that they are properly captured by the approach pursued in §4. For the sake of brevity, we consider the solution of this nonlinear problem only for explicit temporal discretizations.

**SM3.1. Nonlinear least squares formulation.** Ideally, we seek a coarse-grid time-stepping operator \( \Psi \) that minimizes estimates (3.1) for the coarse-grid MGRIT error propagation matrix \( T_\Delta \):

\[
\Psi := \arg\min_{\hat{\Psi} \in \mathbb{R}^{n_x \times n_x}} \| T_\Delta (\hat{\Psi}) \|_2^2 = \arg\min_{\hat{\Psi} \in \mathbb{R}^{n_x \times n_x}} \max_{1 \leq k \leq n_x} \| T_{\Delta, k} (\hat{\Psi}) \|_2^2.
\]

Such minimax problems are, in general, difficult to solve given their non-smoothness. For this reason, we approximate (SM1) with a smoother problem, in which the max-norm is replaced with the two-norm. This yields the following nonlinear least squares problem

\[
\Psi := \arg\min_{\hat{\Psi} \in \mathbb{R}^{n_x \times n_x}} \frac{1}{n_x} \sum_{k=1}^{n_x} \| T_{\Delta, k} (\hat{\Psi}) \|_2^2.
\]

To solve this problem, we use MATLAB’s nonlinear least squares routine, \texttt{lsqnonlin}, which employs the well-known Levenberg–Marquardt algorithm. Again, we only focus on discretizations of (2.1) with periodic boundary conditions, such that the underlying convergence theory of [7] applies. As previously, this also means that the time-stepping operators’ eigenvalues—which are required for evaluation of the objective function in (SM2)—are inexpensive to compute, and are linearly related to the entries in the underlying circulant matrices via the DFT.
SM3.2. Results. Here, we consider the solution of (SM2) for ERK discretizations of (2.1). The default settings are used for MATLAB’s lsqnonlin, except that a maximum of 30 nonlinear iterations is permitted\(^2\). The sparsity patterns for Ψ used in §4.3 are also applied here since they were successful. Likewise, since the solution of weighted linear least squares problem (4.3) was successful in §4, it is passed to lsqnonlin as the initial iterate in all instances. MGRIT iteration counts obtained using the resulting coarse-grid operators are given in Table SM6, where both F- and FCF-relaxation have been tested.

| Scheme | \( n_x \times n_t \) | \( m \) (F-relaxation) | \( m \) (FCF-relaxation) |
|--------|---------------------|------------------------|------------------------|
|        | 2 \(^8\) \times 2\(^{10}\) | 11 7 8 13 10 10 | 10 6 6 6 5 5 |
|        | 2 \(^{10}\) \times 2\(^{12}\) | 12 8 8 14 10 11 | 11 6 6 6 6 5 |
|        | 2 \(^{12}\) \times 2\(^{14}\) | 12 8 8 14 11 11 | 11 6 6 6 5 5 |
| ERK2+U2 | 2 \(^8\) \times 2\(^{14}\) | 18 12 12 14 13 12 | 10 7 7 7 5 6 |
|        | 2 \(^{10}\) \times 2\(^{13}\) | 18 12 13 13 12 12 | 10 7 8 8 6 6 |
|        | 2 \(^{12}\) \times 2\(^{15}\) | 17 12 14 16 15 13 | 10 7 8 8 7 7 |
| ERK3+U3 | 2 \(^8\) \times 2\(^{16}\) | 10 9 9 8 9 6 | 7 5 5 4 4 3 |
|        | 2 \(^{10}\) \times 2\(^{17}\) | 10 9 10 9 11 6 | 7 5 5 5 4 4 |
|        | 2 \(^{12}\) \times 2\(^{19}\) | 10 10 10 10 12 7 | 6 6 5 6 5 4 |
| ERK4+U4 | 2 \(^8\) \times 2\(^{18}\) | 6 8 6 7 7 9 | 5 4 4 4 4 4 |
|        | 2 \(^{10}\) \times 2\(^{20}\) | 7 8 6 7 7 11 | 5 4 4 4 5 5 |
|        | 2 \(^{12}\) \times 2\(^{22}\) | 7 8 7 7 8 13 | 5 4 4 4 5 5 |
| ERK5+U5 | 2 \(^8\) \times 2\(^{20}\) | 4 4 4 6 7 6 | 3 3 3 4 4 3 |
|        | 2 \(^{10}\) \times 2\(^{21}\) | 4 4 4 6 7 6 | 3 3 3 4 4 4 |
|        | 2 \(^{12}\) \times 2\(^{23}\) | 4 4 5 6 7 6 | 3 3 3 4 4 4 |

Table SM6 shows that fast and scalable convergence is consistently obtained with FCF-relaxation; in most instances, F-relaxation, while requiring more iterations, also yields fast convergence and appears to be scalable for the most part. The larger iteration counts resulting from using F- over FCF-relaxation are most pronounced in the lower-order discretizations, with the 2nd-order scheme seeing the largest degradation. For solves in which F- and FCF-relaxation iteration counts are not very different, the algorithm using F-relaxation would likely be faster since an F-relaxation requires roughly half the work of an FCF-relaxation.

The FCF iteration counts from Table SM6 are similar to those in Table 3, where Ψ was the solution of linear least squares problem (4.3). In most cases, the iteration counts in the two tables are almost identical. Even though the iteration counts for the two optimization formulations result in the same or similar iteration counts, they appear, in general, to not be converging to the same solution, as is evidenced by the examples in Figure SM1, suggesting that MGRIT convergence is not very sensitive to the precise optimization problem solved.

Interestingly, for the particular example shown in the right panel of Figure SM1,

\(^2\)One exception here is for ERK2+U2 using FCF-relaxation with \(m = 64\) where the solutions generated resulted in an MGRIT solver whose convergence stalled. Permitting lsqnonlin to use only 10 iterations in this instance appears to resolve this issue.
it looks as if the nonlinear least squares solution for F-relaxation has just truncated \( \Psi_{\text{ideal}} \) within the prescribed sparsity pattern, but closer inspection reveals this is not quite the case. In fact, we find that truncating \( \Psi_{\text{ideal}} \) inside the prescribed sparsity pattern does not result in a scalable solver. The corresponding iteration counts are \{6, 9, 15\} for \( n_x \times n_t \in \{2^8 \times 2^9, 2^{10} \times 2^{11}, 2^{12} \times 2^{13}\} \), which are quite poor compared to the constant iteration count of seven achieved with the nonlinearly determined \( \Psi \) (Table SM6). This is also related to Remark 4.1, that minimizing \( \| \Phi^m - \Psi \|_2^2 \) to which the solution is simply truncating \( \Psi_{\text{ideal}} \)—in some instances leads to a fast solver, but does not appear scalable in general. It is quite surprising that such a small perturbation in the solution (i.e., the perturbation between truncating \( \Psi_{\text{ideal}} \) and the nonlinearly determined \( \Psi \) for F-relaxation) can lead to such drastically different convergence behaviour for MGRIT.

![Diagonal entries from various coarse-grid operators Ψ as a function of their diagonal index, i, for coarsening factor m = 32 and spatial resolution n_x = 2^{12}. Left: ERK1+U1. Right: ERK5+U5. Entries from ideal operators Ψ_{ideal} := Φ^m with magnitude larger than 10^{-3} are shown, as are those from linear least squares solutions (4.3), and so are those of nonlinear least squares solutions (SM2) for both F- and FCF-relaxation.](image)

The results in Tables 3 and SM6 clearly demonstrate that fast and scalable MGRIT convergence is obtainable for explicit discretizations of the advection equation (2.1) with the right choice of coarse-grid operator. Moreover, the fact that the linearly and nonlinearly determined \( \Psi \) lead to such similar MGRIT convergence rates, despite the nonlinear problem arising as more of a direct minimization of error estimates (3.1), indicates that the heuristics developed in §3.1 are accurate, and that they are well captured by the solution of weighted linear least squares problem (4.3).

**SM4. Parallel results: Two-level solvers.** In this section, we present strong parallel scaling results for two-level solvers to accompany the multilevel results from §5. In the setting of two time grids, two effects have to be balanced for optimizing parallel performance. On the one hand, aggressive coarsening with \( m \gg 2 \) reduces the number of coarse-grid points and, thus, the cost of the sequential coarse-grid solve. On the other hand, when using a large coarsening factor, relaxation on the fine grid is performed sequentially over a larger time interval, that is, for more time points. Typically, the fastest runtimes on a given number of processors have been obtained when using a coarsening factor such that the number of coarse-grid points is equal to the number of processors. Figure SM2 shows compute times of two-level MGRIT for \( m = 64 \) coarsening, with dashed lines representing runtimes of sequential time-
stepping for reference purposes. On smaller numbers of processors, time-stepping is faster, demonstrating the computational overhead of the MGRIT approach. This extra work, however, can be effectively parallelized at higher processor counts with good parallel scalability. The crossover point at which it becomes beneficial to use MGRIT over sequential time-stepping is between eight and 64 processors, depending on the discretization and on the stopping criterion. For ERK1+U1, for example, when solving to high accuracy, the crossover point is at 64 processors, while using only eight processors results in a faster compute time than sequential time-stepping for achieving discretization error accuracy. In both settings, the largest speed-up achieved over sequential time-stepping is at 128 processors, where two-level MGRIT is faster by a factor of about 1.4, 3.6, and 5.5 when solving to a residual tolerance of $10^{-10}$, and speed-ups of about 4.1, 4.5, and 4.7 when solving up to discretization error (for the discretizations in the order of increasing accuracy). Note that, considering $m = 64$ coarsening and $2^{13}$ time steps on the fine grid as for the discretizations of orders three and five, the coarse grid consists of 128 time points corresponding to the number of processors for which the largest speed-up is achieved.

![Fig. SM2](image)

**Fig. SM2.** Strong parallel scaling: Runtimes of two-level MGRIT using FCF-relaxation with $m = 64$ coarsening and using time-only parallelism for ERK$p$+U$p$ discretizations on space-time grids of size $2^{12} \times \{2^{14}, 2^{13}, 2^{13}\}$ for $p \in \{1, 3, 5\}$. Left: Fixed residual stopping tolerance of $10^{-10}$. Right: Residual stopping tolerance based on the discretization error. Dashed lines represent runtimes of time-stepping on one processor for reference purposes. Solid red markers represent crossover points.