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Parallelizing Across Time When Solving Time-Dependent Partial Differential Equations

Patrick H. Worley

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Engineering Physics and Mathematics Division

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PARALLELIZING ACROSS TIME WHEN SOLVING TIME-DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

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PARALLELIZING ACROSS TIME WHEN SOLVING TIME-DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

Patrick H. Worley

Abstract

The standard numerical algorithms for solving time-dependent partial differential equations (PDEs) are inherently sequential in the time direction. This paper describes algorithms for the time-accurate solution of certain classes of linear hyperbolic and parabolic PDEs that can be parallelized in both time and space and have serial complexities that are proportional to the serial complexities of the best known algorithms. The algorithms for parabolic PDEs are variants of the waveform relaxation multigrid method (WFMG) of Lubich and Ostermann where the scalar ordinary differential equations (ODEs) that make up the kernel of WFMG are solved using a cyclic reduction type algorithm. The algorithms for hyperbolic PDEs use the cyclic reduction algorithm to solve ODEs along characteristics.

1. Introduction

For many numerical problems in scientific computation, the execution time grows without bound as a function of the problem size, independent of the number of processors and of the algorithm used [40], [43]. In particular, for most linear partial differential equations (PDEs) arising in mathematical physics, the parallel complexity grows as $\log N$, where N is a particular measure of the problem size. The proof is based on deriving upper and lower bounds on the execution time of *optimal parallel algorithms* for multiprocessors with an *unlimited number of processors* and *no interprocessor communication costs.* (Lower bounds for the case when communication costs are not zero can also be calculated [40], [41], [43].) Due to the assumption on the number of processors, these optimal parallel algorithms can have very large serial complexities, and the tightness of the bounds on the parallel execution time for practical algorithms is not established by this analysis.

An analysis of standard numerical algorithms for linear PDEs indicates that growth in the parallel execution time for these algorithms has an important effect when using scaled speed-up models to evaluate multiprocessor performance [42]. In this analysis, there is a strong dichotomy in the nature of the growth in the parallel execution time between algorithms for the solution of time-dependent and time-independent PDEs, *a dichotomy that is not present in the algorithm-independent analysis.* For example, when approximating elliptic PDEs using finite difference or finite element discretizations, the serial complexity is at least $\Theta(N_s)$, where N_s is the size of the underlying grid and $\Theta(x)$ denotes a positive quantity whose leading order term is proportional to x [16, p. 31]. This linear serial complexity can often be achieved using a full multigrid V-cycle algorithm, weighted Jacobi or multi-color Gauss-Seidel relaxation, and local restriction/prolongation operators, which has a parallel complexity of $\Theta(\log^2 N_s)$ on a multiprocessor with $\Theta(N_s)$ processors [2], [3], [5], [11]. So, for these problems, there exists an algorithm whose serial complexity is proportional to that of the best serial algorithm and whose parallel complexity is a polylog function of the serial complexity.

Timestepping methods are commonly used to calculate the time-accurate solution of time-dependent PDEs. For a time-accurate solution, the solution is required at a sequence of times $\{t_i \mid i = 0, \ldots, N_t\}$, where $t_{i-1} < t_i$ and $t_i - t_{i-1}$ is small enough to allow accurate interpolation of the solution at all times in between. Timestepping algorithms calculate the approximate solution for each time level in sequence, calculating the solution at time t_i from the approximate solution at times $t_j, j < i$. Standard timestepping algorithms based on finite difference or finite element discretizations of hyperbolic and parabolic PDEs have serial complexities that are linear in the number of space-time locations where the solution function is approximated. Thus, the serial complexity is $\Theta(N_s \cdot N_t)$, where N_s is the size of the underlying grid at a fixed time and N_t is the number of time levels. The calculation of each time level is usually

easily parallelized, but the time direction in a timestepping algorithm is inherently sequential. Thus, the parallel complexity is always at least $\Theta(N_t)$, i.e. not a polylog function of the serial complexity. (Variants of the standard timestepping algorithms have been proposed that begin the calculation for later time levels before the current time level is finished [12], [30], [39], but these algorithms do not alter the sequential nature of the time direction.) This paper addresses the question of whether good serial algorithms for time-dependent PDEs are intrinsically less parallel than good serial algorithms for time-independent PDEs. We pose the question in the following form:

For a given time-dependent PDE, is there a numerical algorithm for the time-accurate approximation of the solution with the properties:

(1) *Let $C_s(N)$ be the serial complexity of the algorithm for a problem of size N, and let $C_{s,\ \mathrm{opt}}(N)$ be the serial complexity of the best known serial algorithm for this problem. Then $C_s(N) = \Theta(C_{s,\ \mathrm{opt}}(N))$.*

(2) *The algorithm can be parallelized in the time direction as well as the spatial directions, so that the achievable parallel complexity given an unlimited number of processors, $C_p(N)$, satisfies $C_p(N) = \Theta(\log^\gamma C_s(N))$ for some finite constant γ.*

In this paper,[1] we describe a class of algorithms that have properties (1) and (2) for a large class of linear parabolic PDEs. Not only does this class of algorithms answer the above theoretical question, it may also have practical applications on massively parallel multiprocessors. We also briefly describe a different class of algorithms with properties (1) and (2) for a particular class of linear hyperbolic PDEs.

2. Parabolic PDEs

2.1. Waveform relaxation

Waveform relaxation is a technique for solving systems of ordinary differential equations of initial-value type [26], [29]. It is based on applying standard point and block iterative methods for the solution of linear systems [37] to the solution of a system of ODEs. For example, let A be an $n \times n$ matrix, and consider the problem $dU/dt + AU = F$, where U and F are vector functions of time. Then the kth step of a Jacobi-based iterative method for the solution of this system is

$$\frac{d}{dt}U^{(k)} + DU^{(k)} = F + (D - A)U^{(k-1)}, \tag{1}$$

[1] An earlier version of this paper appears in the Proceedings of the Fifth SIAM Conference on Parallel Processing for Scientific Computing.

where D is the diagonal of A. Thus, each step of the method involves the solution of n independent scalar ODEs. The decoupling of the system allows different discretizations and timesteps to be used for each of the ODEs, which can lead to significant savings for some applications.

To solve parabolic PDEs, the spatial derivatives are discretized to generate a semi-discrete problem and the resulting system of ODEs is solved using waveform relaxation. Miekkala and Nevanlinna have analyzed the convergence of waveform relaxation for linear operators [28]. They showed that, for linear PDEs of the form $u_t + Lu = f$ where L is an elliptic operator and for standard spatial discretizations, the convergence rates for Jacobi and Gauss-Seidel iterations for the semi-discrete problem are similar to those for the analogous linear system.

2.2. Waveform relaxation multigrid

Let L_h represent the discrete operator generated by discretizing an elliptic operator L. The correspondence between the convergence rate of waveform relaxation applied to $dU/dt + L_h U = F$ and the convergence rate of the analogous matrix iterative method applied to $L_h U = F$ has two immediate implications. First, the convergence rate is too slow for waveform relaxation to be competitive with standard timestepping algorithms. Second, multigrid techniques may be effective at accelerating convergence of the iteration.

Multigrid acceleration has been analyzed by Lubich and Ostermann [27]. Among their results, they showed that full multigrid performance can be achieved for the semi-discrete problem if L_h is symmetric positive definite, and either L_h has constant diagonal entries, in which case weighted Jacobi relaxation is used, or L_h has the form

$$\begin{pmatrix} D_1 & B \\ A & D_2 \end{pmatrix}, \tag{2}$$

where D_1 and D_2 are diagonal, in which case Gauss-Seidel relaxation is used. Note that this latter matrix structure commonly occurs when using a red-black ordering with standard finite difference stencils. They also show that full multigrid performance can be achieved for the fully discrete problem (i.e. linear serial complexity) if, in addition to the above conditions, all ODEs are discretized by the same method, the time direction is not coarsened, and the ODE solver is an A-stable linear multistep or Runge-Kutta method. Full multigrid performance also holds for $A(\alpha)$-stable linear multistep or Runge-Kutta methods for suitably large α. Note that all of these conditions are sufficient, but not necessary.

This *waveform relaxation multigrid* algorithm has been tested extensively [32], [33], [34], [35], [36], and has been shown to work well for a variety of parabolic problems, both linear and nonlinear, on both serial and parallel computers.

2.3. Waveform relaxation multigrid cyclic reduction

The waveform relaxation multigrid algorithm is normally implemented in a fashion that is still intrinsically sequential in the time direction. But computation in the time direction only involves solving linear scalar ODEs. If the ODEs are solved using a linear multistep method with a statically determined timestep, then each ODE solution corresponds to the solution of a banded lower triangular matrix equation, or, equivalently, a linear recurrence. Parallelizing linear recurrence equations has been studied extensively [9], [14], [15], [21], [22], [23], [24], [31]. In particular, if a cyclic reduction approach is used to parallelize the linear recurrence, then parallelism is introduced without increasing the order of the serial complexity. For example, if a two-level scheme, like backward Euler or Crank-Nicolson, is used to discretize the scalar ODE, then a lower bidiagonal matrix equation must be solved. Cyclic reduction combines even numbered equations with odd numbered equations to generate a new bidiagonal matrix equation of half the size. If the original matrix has the form

$$\begin{pmatrix} a_{11} & & & \\ a_{21} & a_{22} & & \\ & a_{32} & a_{33} & \\ & & a_{43} & a_{44} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix}, \tag{3}$$

then one step of the cyclic reduction algorithms generates a new matrix equation of the form

$$\begin{pmatrix} a_{22} & \\ -\frac{a_{43}}{a_{33}} a_{32} & a_{44} \end{pmatrix} \cdot \begin{pmatrix} x_2 \\ x_4 \end{pmatrix} = \begin{pmatrix} f_2 - \frac{a_{21}}{a_{11}} f_1 \\ f_4 - \frac{a_{43}}{a_{33}} f_3 \end{pmatrix}. \tag{4}$$

The solution vector of the smaller system is identical to the even-numbered elements of the solution vector of the original matrix equation. This process is repeated until only two equations are left, at which time the two-by-two linear system is solved. The solution values for the small system are then used to calculate the unresolved values in the next larger linear system. For example, in (3), $x_3 = (f_3 - a_{32}x_2)/a_{33}$, which can be calculated immediately since x_2 was determined when solving the smaller system. By repeating this process, the solution to the original matrix equation is calculated. Note that each step of the reduction stage is perfectly parallel, in the sense that combining each pair of equations is independent. Similarly, injecting solution values into the next larger system and solving for the unresolved variables can be done independently for each unresolved variable. Thus, cyclic reduction allows us to parallelize the time direction.

If a k-step linear multistep algorithm is used to solve the ODE, then the banded lower triangular matrix defining the linear recurrence has a bandwidth of k. The cyclic reduction

algorithm again halves the number of equations at each step, but now k consecutive equations are needed to transform the dependencies in a given equation from the previous $k-1$ values in the current matrix equation to the $k-1$ previous values in the new smaller system. As before, this process is continued until only k equations are left. If $k > 2$, then solving the $k \times k$ system and injecting the solution back into the next larger system does not decouple the calculation of the unresolved variables. Instead, it produces a new banded lower triangular matrix equation to solve, one whose bandwidth is $\lceil k/2 \rceil$. Repeatedly applying the cyclic reduction algorithm continues to halve the bandwidth until all of the unresolved variables are calculated, at which time they can be injected into the next larger system to reduce its bandwidth.

The cyclic reduction algorithm is more expensive than the standard serial algorithm, but the complexity is still $\Theta(N_t)$ for each ODE solution (if k is independent of N_t). For example, for a two-level scheme, the serial complexity of the standard algorithm is $3N_t$, while for the cyclic reduction algorithm it is $5N_t$ or $7N_t$, depending on whether certain values are precomputed. For a three-level scheme, the complexity of the standard algorithm is $5N_t$, compared to $11N_t$ or $21N_t$ for the cyclic reduction algorithm. As long as the complexity of the ODE solver is $\Theta(N_t)$, the waveform relaxation multigrid algorithm remains an $\Theta(N_s \cdot N_t)$ complexity algorithm.

The parallel complexity of the cyclic reduction algorithm is a function of the number of time levels used in the discretization of the ODE. For a k-level scheme, it is $\Theta(\log^\gamma N_t)$, where $\gamma = \lceil k/2 \rceil$. Thus, including the parallel cyclic reduction algorithm in a parallel waveform relaxation multigrid algorithm based on weighted Jacobi or red-black Gauss-Seidel iteration results in a total parallel complexity of the form $\Theta(\log^2 N_s \cdot \log^\gamma N_t)$, which is worse than for elliptic problems, but is still polylog.

2.4. Numerical Results

Parallel implementations of multigrid and cyclic reduction have been discussed elsewhere. See [11], [19], and [38] for pointers to the literature. In this section, we verify the predicted linear serial complexity of the waveform relaxation multigrid algorithms for a specific example problem.

We solved the heat equation $u_t + \nabla u = f$ on the unit square $[0,1] \times [0,1]$ in the time interval $[0,1]$ using Dirichlet boundary conditions. Standard centered differencing was used to discretize the spatial derivatives. Crank-Nicolson, a two-level scheme, and the 2nd order backward difference formula (BDF), a three-level scheme, were used to discretize the time derivative. The same timestep and spacestep were used in the discretization, $\sqrt{N_s} = N_t$, and a sequence of problem sizes was examined.

Three algorithms were tried: waveform relaxation mutigrid with the cyclic reduction ODE solver (WFMGCR), waveform relaxation mutigrid with the standard ODE solver (WFMG), and

a timestepping algorithm that uses multigrid at each timestep. The convergence of the multigrid algorithm was essentially identical for all three algorithms, and four full V-cycle multigrid cycles, with 1 relaxation sweep before and after each coarse grid correction, was sufficient to identify convergence (small residual and little change between successive iterates) for all problem sizes and forcing functions tried. The approximate solutions were also essentially identical, indicating that the cyclic reduction algorithm is no less stable (for these problems) than the standard ODE solver. The numbers of floating point operations (flops) required to solve the problems are displayed in Figures 1 and 2. The data indicate linear growth in complexity for all three methods, with WFMGCR being somewhat more expensive than WFMG because of its more expensive ODE solver.

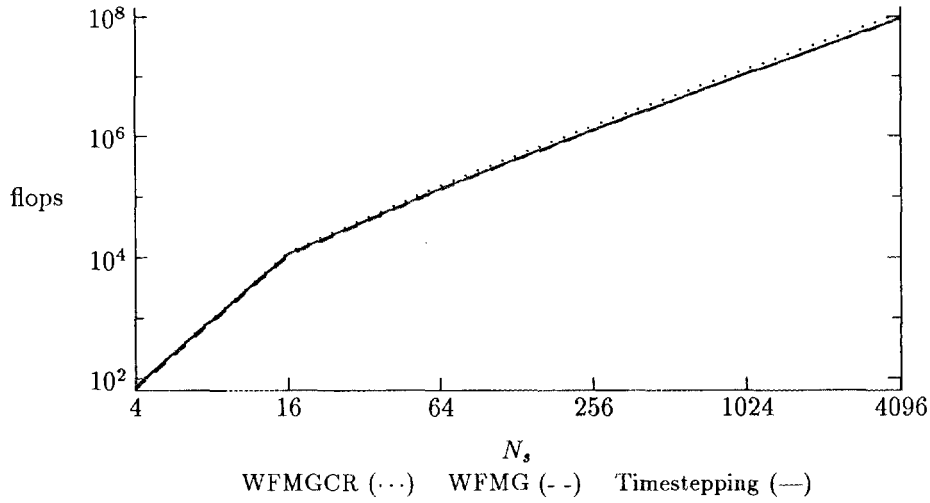

Figure 1: Serial complexity for Crank-Nicolson time discretization.

2.5. Discussion

Using cyclic reduction with the waveform relaxation multigrid algorithm has the desired properties (linear serial complexity and polylog parallel complexity) for all problems for which (a) the waveform relaxation multigrid algorithm has a linear serial complexity when using a relaxation technique that can be efficiently parallelized, like Jacobi or multi-color Gauss-Seidel, and (b) cyclic reduction is a stable algorithm for solving the linear recurrences arising from discretizing the scalar ODEs. Both theory and empirical evidence indicate that (a) is true for a large class of parabolic problems, both linear and nonlinear. While some work on the stability of parallelizing recurrence equations has been done [21], [31] and the numerical examples described here give no indication of stability problems, more work must be done to establish the

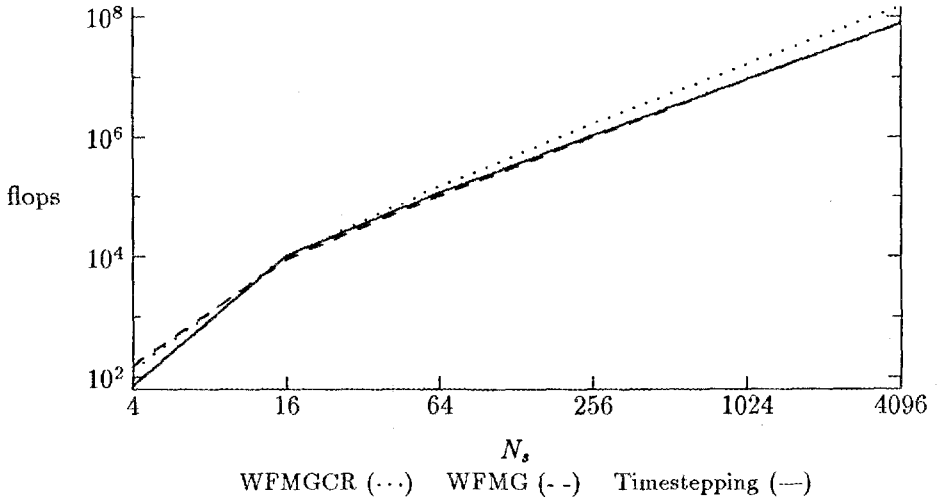

Figure 2: Serial complexity for second order BDF time discretization.

stability of this algorithm, especially when the bandwidth of the recurrence (k) is large. This is especially true given the stability problems of the straightforward implementation of cyclic reduction for elliptic problems [8].

When properties (a) and (b) hold, we have shown the algorithm to have an achievable parallel complexity of $\Theta(\log^2 N_s \cdot \log^\gamma N_t)$, where $\gamma = \lceil k/2 \rceil$. This is higher than that for elliptic problems, and the question arises as to whether it can be decreased. There is some hope since it is normally not necessary to solve the "subproblems" exactly in a multigrid solver. The simplest approach is to use Jacobi iteration to approximately solve the banded triangular systems, instead of using cyclic reduction. This is essentially the method of Hackbusch [13], which has been shown to lead to an efficient parallel algorithm for many applications, if some care is taken in choosing the discretization [1], [6], [7], [17], [18]. But the following argument shows that the total number of Jacobi iterations used to approximate the solution of the triangular systems over the course of the algorithm must increase at least linearly as a function of N_t.

Consider solving for the solution at a given location in the space-time grid. As the error due to the discretization decreases, and N_t increases, data throughout an increasing portion of the domain of dependence of the solution operator for this location must be sampled to accurately approximate the solution. Since this domain is independent of N_t, and since some fixed fraction α of the N_t grid points used to approximate the scalar ODE falls in this domain, at least αN_t Jacobi iterations are required for the data at these grid points to be used in approximating the solution at the given location. Thus, asymptotically, the parallel complexity will have a term that grows like N_t. The same argument applies to other point iterative methods that

might be used to solve the triangular systems in parallel. Note that this is not necessarily a condemnation of Hackbusch's method since this growth as a function of N_t can be very small, and may not show up for realistic sized problems.

The obvious approach to avoiding the problem indicated above is to coarsen the grid in time (as well as space) during the multigrid process. In this way, data from more distant grid points can propagate through the coarse grids. Unfortunately, the theory of Lubich and Ostermann does not hold in this situation, and experiments indicate that naive implementations of this approach do not work. Local mode (Fourier) analysis for the example problem and discretizations described in §2.4 confirm the experimental evidence, that coarsening in time does not work, but more sophisticated discretizations, possibly differing between grids, may still allow the time direction to be treated in an analogous way to the spatial directions [4]. In summary, whether or not the parallel complexity can be further reduced, without a corresponding increase in the serial complexity, is not yet known.

2.6. Generalizations

The *waveform relaxation multigrid cyclic reduction* algorithm described above was motivated by the theoretical question introduced in §1. The following generalizations are motivated by practical issues.

Fine grain parallel algorithms By imitating Hockney's PARACR algorithm [15], we can lower the parallel complexity of the parallel cyclic reduction algorithm to $\Theta(\log N_t)$, independent of the length of the recurrence, without increasing the number of processors needed. The trick is to modify all equations at each reduction step. Thus, after $\log_2 N_t$ steps, there are N_t/k independent $k \times k$ systems whose solutions solve the original problem. While the resulting algorithm has a serial complexity of $\Theta(N_t \log N_t)$, this is unimportant on a multiprocessor with $\Theta(N_s \cdot N_t)$ processors.

Coarse grain parallel algorithms - I By imitating the blocked cyclic reduction algorithm discussed in [19] and [20], the communication cost can be reduced to a manageable size for distributed memory multiprocessors. For example, if P_t processors are assigned to the solution of an ODE, the blocked algorithm generates a $P_t \times P_t$ linear system whose solution introduces P_t-way parallelism into the rest of the calculation.

Coarse grain parallel algorithms - II Since each relaxation in the multigrid algorithm involves the solution of many ODEs, much of the analysis used in determining how best to parallelize ADI algorithms for elliptic problems applies immediately [19], [20]. In particular, this analysis addresses the issue of whether to move data for a single ODE to a single processor

and use a fast serial algorithm or to use a cyclic reduction algorithm to parallelize the ODE solution, attempting to overlap communication with computation since parts of many ODE calculations may be assigned to the same processor.

Coarse grain parallel algorithms - III Selectively exploiting parallelism in time can alleviate the inefficiency of solving on coarse grids in the multigrid algorithm. For example, the cyclic reduction algorithm might be used only on coarse grids, when processors have been idled by the coarsening.

3. Hyperbolic PDEs

While waveform relaxation can be used to solve hyperbolic PDEs, multigrid does not accelerate the convergence, and the serial complexity of the resulting algorithm is not $\Theta(N_s \cdot N_t)$. But the same approach to parallelizing in time can be applied to any algorithm whose computational kernel is solving a linear scalar ODE. In this section we briefly describe such an algorithm for constant coefficient hyperbolic PDEs that can be written in the form

$$U_t + \sum_{i=1}^{d} A_i \cdot U_{x_i} = F, \tag{5}$$

where the $n \times n$ matrices $\{A_i\}$ can be simultaneously diagonalized. Here, the problem is defined in d space dimensions and F is a function of both $\bar{x}$ and t, where $\bar{x} = (x_1, \ldots, x_d)$.

Let T be the matrix that diagonalizes $\{A_i \mid i = 1, \ldots, d\}$, $TA_iT^{-1} = \Lambda_i$. Define $V = TU$ and $G = TF$. Then (5) can be written as

$$V_t + \sum_{i=1}^{d} \Lambda_i \cdot V_{x_i} = G. \tag{6}$$

Equation (6) is actually n independent scalar PDEs of the form

$$v_t + \sum_{i=1}^{d} \lambda_i v_{x_i} = g, \tag{7}$$

each of which can be solved be solved by integrating the ODE

$$\frac{d}{dt} v(\lambda_1\xi_1 + t, \ldots, \lambda_d\xi_d + t, t) = g(\lambda_1\xi_1 + t, \ldots, \lambda_d\xi_d + t, t) \tag{8}$$

along the characteristic defined by the set of equations $\{\xi_i = x_i - \lambda_i t \mid i = 1, \ldots, d\}$ for each point $(\xi_1, \ldots, \xi_d)$ in the problem domain [10], [25]. For a numerical algorithm, we would specify a grid in the space-time domain and only track characteristics that exit the space-time domain

at a grid point. To recover the desired variables requires interpolating from characteristics back to the desired space-time grid, and calculating $T^{-1}V$ at each grid location. Since this overhead is a linear function of the number of grid points, the serial complexity of the resulting algorithm is still linear. Both the interpolation and the inversion are "local" processes, and all ODE calculations are independent. Therefore, the parallel complexity of the overall algorithm is $\Theta(\log^{\gamma} N_t)$ when using cyclic reduction, where γ is again determined by the number of levels in the discretization of the ODE.

Note that the form of (5) is very general. For example, the wave equation $u_{tt} - u_{xx} = f$ can be rewritten as

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix}_t + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}_x = \begin{pmatrix} f \\ 0 \end{pmatrix}, \tag{9}$$

where $v_1 = u_t$ and $v_2 = u_x$. After applying the above algorithm to solve for v_1 and v_2, u can be recovered by solving the ODE $u_t = v_1$ for each spatial grid point, using the parallel cyclic reduction algorithm as before. This extra step alters neither the order of the serial complexity nor the order of the parallel complexity.

4. Conclusions

The algorithms described in this paper establish that major classes of linear time-dependent PDEs can be solved in polylog parallel time without giving up linear serial complexity. Beyond the theoretical question, WFMGCR has promise as a practical parallel algorithm, as indicated in §2.6, since WFMG is a competitive serial algorithm for many applications. Additionally, WFMGCR can be used for nonlinear problems since many multigrid solvers automatically linearize the ODEs.

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