Parallel-in-Space/Time Method for Explicit Time-Marching Scheme

Yen-Chen Chen[1,a)] Kengo Nakajima[1,b)]

Abstract: Numerical PDE solvers require heavy computation power to solve and efficient parallel processing to accelerate. The traditional methods parallelize only in the spatial dimensions but not the time dimension. However, this limited the scalability we can do by parallel computation. Therefore, several Parallel-in-Space/Time (PinST) methods are proposed to accelerate PDE solvers further. One of the famous PinST methods is MGRIT method[1]. The MGRIT method takes advantages of the multigrid method and applied it on both the space dimensions and the time dimension, which has been proved to work well on linear problems. Another method is the Time Segment Correction (TSC), which works more stable on highly non-linear problems. However, the number of converge iteration for TSC grows with time dimension size, therefore requires more computation on large-scale problems. In the present work, we propose a new PinST method targetting explicit time-marching schemes.

Keywords: Parallel-in-time, PinT, PinST, Multigrid, MGRIT, PDE, explicit scheme

1. Introduction

Since the parareal[2] method in 2001, parallel-in-time methods have been proposed to accelerate PDE solvers further. One of the most popular and effective parallel-in-time methods is the *multigrid reduction in time* (MGRIT)[1] method. In the past few years, the MGRIT is broadly used and studied[6], [7], [8], [9]. The MGRIT method is proven to help solve several PDE applications, and the iteration number does not grow with problem size. However, the MGRIT method does not work with explicit time-marching scheme. Due to the restriction of the CFL condition for explicit methods, coarse grids in MGRIT are very unstable with explicit schemes. Nevertheless, some of the physics simulation like sonic wave still prefers explicit time-marching over implicit time-marching methods. This research aims to develop a explicit MGRIT method that works reasonably fast but would not get numerically unstable at coarser grids.

In the following sections, first, we will give some basic knowledge of the multigrid reduction in time (MGRIT) method in Section 2. Then, we explain our Explicit MGRIT method in Section 3. After that, in Section 4, we do numerical experiments on two one dimensional methods with different explicit schemes. One of the examples is heat transfer with the forward Euler method, and the other example is advection with the Lax-Wendroff method. At last, we have conclusion in Section 5 and future work in Section 6.

1 The University of Tokyo, Bunkyo-ku, Tokyo 133–8656, Japan
a) yenchen_chen@mist.i.u-tokyo.ac.jp
b) nakajima@cc.u-tokyo.ac.jp

2. MGRIT

The multigrid reduction in time (MGRIT) method is a parallel-in-time method inspired by the multigrid method. The MGRIT method, compared to the parareal method, supports deeper hierarchy and has more algorithmic flexibility.

2.1 The multigrid method

The multigrid method is an iterative solver commonly used to solve large linear systems. The multigrid method creates a multiple level hierarchy from fine mesh grids to coarse mesh grids. A multigrid method is composed of four components, relaxation, restriction, prolongation (interpolation), and coarse operation.

- Relaxation: Solve on the current grid with iterative solvers.
- Restriction: Restrict from fine grid to coarse grid.
- Coarse operation: Solve on the coarse grid.
- Prolongation: Update results on the coarse grid back to the fine grid.

The most important feature for the multigrid is that the iteration number of the multigrid method does not grow with the problem size, unlike traditional iterative solvers like the Jacobi/Gauss-Seidel methods and ICCG solver.

2.2 The MGRIT method

The MGRIT method is first proposed in [1]. The MGRIT method is inspired by the multigrid method. The MGRIT method sees the time dimension like other space dimensions.

The coarse time grids are also extracted from the original time grid. The MGRIT method does not solve the time steps sequentially. Instead, it solves through all time steps at the same time and by every iteration, reduce the error on the results of all time steps. The algorithm of the MGRIT method is shown in Algorithm 1.

Algorithm 1: MGRIT(l)

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if l is the coarsest level L, then
    Solve coarse-grid system A_L u^(L) = g^(L)
else
    Relax on A_l u^(l) = g^(l) using FCF-relaxation.
    Compute and restrict residual using injection.
      g^(l+1)=R_1(g^(l) − A_l u^(l))
    Solve on the next level MGRIT(l+1)
    Correct using interpolation u^l ← u^l + P u^(l+1)
end
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The advantage of the MGRIT method is that, as it has the structure of a multigrid method, the iteration number does not grow with the problem size. In the previous rearch[1], the MGRIT method is proved to work well on solving PDE problems with implicit time-marching schemes. However, to our best knowledge, there is not yet successful research on the MGRIT method with explicit time-marching schemes. In the next section, we propose an explicit MGRIT method which solves PDE problems by the MGRIT method with explicit time-marching schemes.

3. Explicit MGRIT scheme

In previous research for MGRIT[1], MGRIT with explicit time-marching schemes is said to be numerically unstable and hard to converge. In early 2019, Krzysik, O. A. et al[10] studied the convergence of the MGRIT method on the linear advection equation. The research concludes that the MGRIT method has a convergence problem with advection equations since it violates the CFL limits at the coarse grid. In this section, we will explain the reason why explicit MGRIT fails easily, and we will propose our explicit MGRIT algorithm. In Section 4.2, we will also test our method on one dimension advection equation.

3.1 CFL condition

The most significant problem for explicit schemes is that they are restricted by the Courant-Friedrichs-Lewy condition (CFL condition)[3]. The solution of an explicit scheme is proved to be unstable if the Courant number is to be more than 1. In order to apply explicit method successfully, one has to choose mesh size and time step adequately such that the Courant number is less than 1. The Courant number can be derived from the Von Neumann stability analysis[4], [5]. For example, the Courant number for one-dimensional advection is $\frac{v\Delta t}{\Delta x}$, where Δt is the time step, Δx is the mesh size, and v is the flow velocity.

3.2 Our method

As we want to use explicit time-marching scheme in MGRIT, the most notable difference with that of implicit scheme is that we don't use iterative solvers like Jacobi or Gauss-Seidel as relaxation methods. We also have to change the way we pick up coarse grids to prevent violating the CFL condition. For the initial condition, since we can also use an explicit scheme to update values from the last time step. We start by initializing all time step by the initial condition. The four multigrid components for our explicit MGRIT method is defined as follows:

- Relaxation: We explicitly march one step on every time step in parallel.
- Restriction: Similar to the multigrid method, we pick out coarse grids with a specific ratio. However, the ratio for picking coarse grids on the x-grid should be the same as that on the time grid.
- Coarse operation: For every level except the coarsest, we solve by explicit MGRIT method on the coarse grid, on the coarsest level, we do nothing.
- Prolongation: We update the coarse grid results on the corresponding position on the fine grid and all the fine grids between two coarse grids by the coarse grid at the front.

The most important part of the method is that we restrict the x grid and the time grid at the same time, such that the Courant number does not change. As shown in Figure 1, the coarse grid is chosen from both x dimension and time dimension. In this research, we coarsen the x-grid and the time grid with the same ratio. For example, if we look at the Courant number of advection:

$$C = \frac{v\Delta t}{\Delta x}$$

$$C' = \frac{v(r\Delta t)}{r\Delta x} = \frac{v\Delta t}{\Delta x} = C$$

where C is the Courant number, C' is the Courant number on the coarse grid, v is the flow velocity, r is the fine grid / coarse grid ratio, Δt is the time step and Δx is the grid size. We can see that the Courant for every coarse layer would not violate the CFL condition. Further detail on advection and the numerical results can be found in Section 4.2.

For prolongation, if we only update the coarse grid as the multigrid method. As explicit schemes still take the results from the neighbor fine grids of the coarse grids for relaxation, the update would be affected by the non-updated points. The result is that the convergence will be slow down by these fine grids. By updating on all fine grid with the coarse grid in the front, we can speed up the convergence for the explicit MGRIT method.

3.3 Algorithm

Algorithm 2 shows the detailed algorithm of the proposed method. In the algorithm, function f can be replaced by any explicit time-marching scheme. In Sections 4.1 and 4.2, we will show results of the explicit MGRIT algorithm with forward Euler and Lax-Wendroff, respectively.

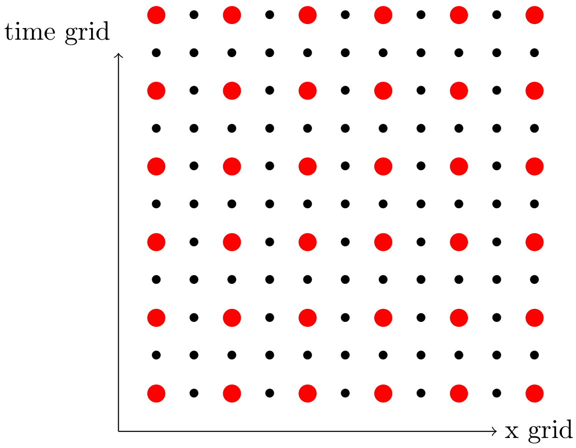

Fig. 1 We take coarse grid from the x grid and the time grid such that the explicit scheme doesn't violate the CFL condition limit. The small black dots represents the fine grids and the large red dots represents the coarse grid.

Algorithm 2: Explicit_MGRIT(l)

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if *l is the coarsest level L,* **then**
  return
else
  Compute next step by explicit time-marching $u^{(t+1)} \leftarrow f(u^{(t)})$.
  Restricted on coarse space/time grids
  Solve on the next level Explicit_MGRIT(l+1)
  Correct on coarse grids.
  Compute next step by explicit time-marching $u^{(t+1)} \leftarrow f(u^{(t)})$.
end

3.4 Theoretical computational time

The MGRIT method is known that when one can parallelize the algorithm efficiently if one has enough computing resource. Consider the situation that we want to compute the result after N time steps, and assume that the computation time of one explicit time-marching is X. We want to compare the theoretical computation time of the explicit MGRIT method to the sequential method. Figure 2 shows the computation time comparison between the time-stepping method and the MGRIT method on 1D nonlinear heat transfer by FDM. Since the explicit MGRIT method is highly parallelizable, we can reduce computational time by adding more processors. We can see that one iteration of an explicit MGRIT method would be faster than the sequential method if we have enough processors. If we have enough processors, the explicit MGRIT would be faster than the sequential method.

4. Numerical Results

In the present work, two examples are used to examine the performance of the explicit MGRIT algorithm. One is a one-dimensional heat transfer example with forward Euler as an explicit scheme. The other is one-dimensional advection of a sine wave with Lax-Wendroff as an explicit scheme. The numerical results show that both examples with different explicit time-marching schemes can be successfully deployed to the explicit MGRIT method and converge to a similar result as the sequential explicit methods.

4.1 Heat transfer

A general one-dimensional heat transfer (assuming no convection, mass transfer, or radiation), can be described in the following form.

$$\rho c\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}(\lambda\frac{\partial T}{\partial x}) + Q$$

where T is temperature, t is time, x is position, ρ is density, c is heat capacity, λ is thermal conductivity, and Q is the heat source. This equation is derived from the first law of thermodynamics (conservation of energy).

In order to simplify the problem, we assume that ρ, c, λ are all 1. We can then write the following:

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + Q$$

Also, for implementation, we assume the initial condition:

$$T(x, t = 0) = 0 \quad \forall x$$

Furthermore, boundary conditions (Dirichlet at the start, Neumann at the end):

$$T(x = 0, t) = 0 \quad \forall t$$

$$\frac{\partial}{\partial x}T(x = x_{end}, t) = 0$$

Finally, we set the number of uniform heat source $Q = \mathbf{1}$.

$$Q(x, t) = 1 \quad \forall x,\ t$$

Then, we get an easy 1D heat transfer example.

$$\frac{\partial \mathbf{T}}{\partial t} = \frac{\partial^2 \mathbf{T}}{\partial x^2} + \mathbf{Q},$$

$$\begin{cases} \mathbf{T}(0, t) = 0 \\ \frac{\partial}{\partial x}\mathbf{T}(x_{end}, t) = 0 \end{cases} \quad \forall t, \quad \& \quad \mathbf{Q} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

Initial condition:

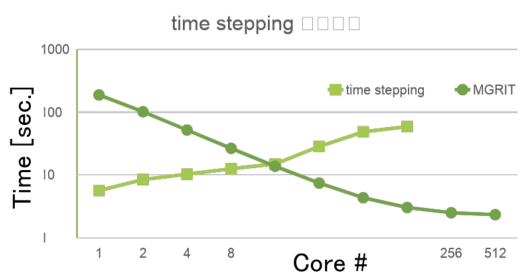

Fig. 2 Comparison of MGRIT and Time-Stepping on Parallel Computing 1D Nonlinear Heat Trasfer by FDM. Refer from Takafumi Fujita, MS Thesis, Graduate School of Information Science and Technology, The University of Tokyo, 2017

$$\mathbf{T} = \mathbf{T}(x, 0) = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}$$

On a closed line $[0, 10]$, we take uniform x-grids with mesh size $\partial x = 0.1$. We set time step $\partial t = 0.001$. We compare the results of sequential forward Euler method and explicit MGRIT at the 60th time step. The explicit MGRIT method we applied here has two layers, one fine grid, and one coarse grid. Figure 3 shows the update progress and the result of the explicit MGRIT method on this example. The results of sequential forward Euler is also shown in Figure 3. We can see that after 11 iterations, the result of the MGRIT method converged to the line overlapping with the sequential method.

We have shown that explicit MGRIT works on the simplest example, the one-dimensional heat transfer, in the next section, we want to try the explicit MGRIT method on advection.

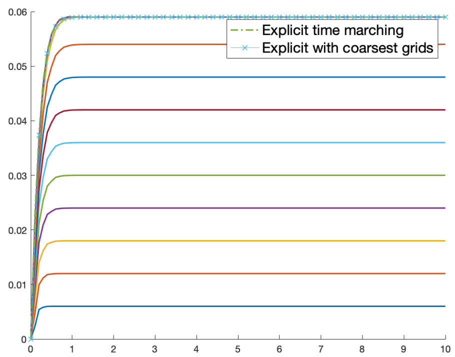

Fig. 3 MGRIT with forward Euler on heat transfer example. From button to top shows the update path of the explicit MGRIT iteration in each iteration. The explicit MGRIT method converged after 11 iterations. one sequential forward Euler result on the fine grid and one on the coarse grid are also drawn on the graph.

4.2 Advection of sine wave

A one-dimensional advection can be described in the following form.

$$\frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x}$$

where u is a scalar field $u(x, t)$, t is time, x is position, and v is the velocity of the flow. For this example, we want to observe the advection of a sine wave. Also, for simplification, we set the velocity $v = 1$. We thus get the following problem statement.

$$\frac{\partial u}{\partial t} = -\frac{\partial u}{\partial x}$$

Initial condition:

$$u(x, 0) = \begin{cases} 0 & 0 \le x \le 50, 110 \le x \le 300 \\ 100[\sin(\pi\frac{x-50}{60})] & 50 \le x \le 110 \end{cases}$$

Figure 4 shows the initial condition of the sine wave. The sine wave will move towards the right with velocity $v = 1$. For the advection example, we use the Lax-Wendroff as the explicit time-marching scheme.

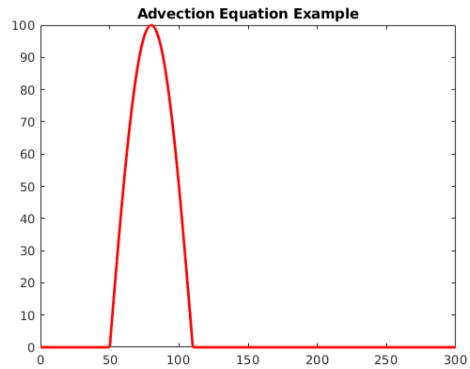

Fig. 4 The initial condition of the target sine wave of the advection example

On a closed line $[0, 300]$, we take uniform x-grids with mesh size $\partial x = 1.25$. We set time step $\partial t = 1$. Under this condition, the Courant number

$$C = \frac{v\Delta t}{\Delta x} = \frac{1 \times 1}{1.25} < 1$$

Thus, the explicit scheme on the fine grids would be stable. Since we pick up coarse grids in x-dimension and time dimension by the same ratio, the explicit scheme on the coarse grids would also be stable. We try to solve the result of the 60th time step. Figure 5 shows the result of explicit MGRIT after 11 iterations compare to sequential Lax-Wendroff on the fine grid and the coarsest grid. We can see that three lines overlap on the hump. This result shows that explicit MGRIT with Lax-Wendroff can derive the result successfully. We can also see that three lines differ at the small tilde before the hump and the line of the explicit MGRIT method is between the line of the fine grid sequential and the coarsest grid sequential result. We can say that the result of the explicit MGRIT is bounded by the sequential results on the fine grid and that of the coarsest grid.

Figure 6 shows the same experiment and the same result of Figure 5, however, the results after every explicit MGRIT iterations are recorded and drawn on the figure. We can see that the wave is updated from left to right, while the peak of the hump drops for each iteration. This amplitude drop is because we update every step by the results of a coarser x-grid. The fine grids, which are not fully updated, has a slightly smaller value than it should be as every explicit time-marching step takes this slightly wrong value to update the next step. However, the correct still can be propagated from the front and fixed after the previous coarse time grid

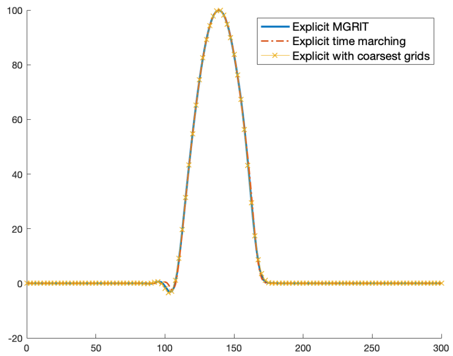

Fig. 5 Explicit MGRIT result compare to sequential Lax-Wendroff method. The blue line represents the result of the explicit MGRIT method with Lax-Wendroff as explicit scheme. The red dashed line represents the result by sequential Lax-Wendroff method on the fine grid (both x grid and time grid). The yellow line with crosses represents the result by sequential Lax-Wendroff method on the coarsest grid (both x grid and time grid).

has reached its convergence point. As shown in Figure 6, the amplitude is corrected after the 11th iteration.

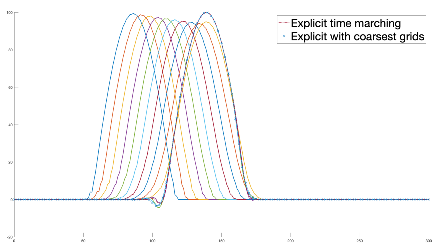

Fig. 6 MGRIT with Lax-Wendroff on advection example. From left to right shows the update path of the explicit MGRIT iteration in each iteration. The explicit MGRIT method converged after 11 iterations. one sequential Lax-Wnedroff result on the fine grid and one on the coarse grid are also drawn on the graph.

Figure 7 shows the result of the advection example with two coarser layers. We can see that compare to Figure 6, it converges faster. The three-layer explicit MGRIT method converged after seven iterations.

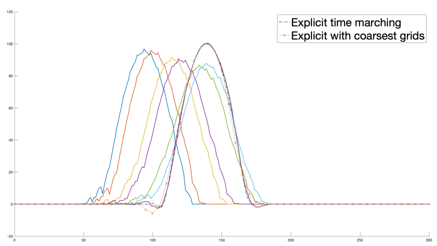

Fig. 7 3 level MGRIT with Lax-Wendroff on advection example. From left to right shows the update path of the explicit MGRIT iteration in each iteration. The explicit MGRIT method converged after 7 iterations. one sequential Lax-Wnedroff result on the fine grid and one on the coarse grid are also drawn on the graph.

5. Conclusion

In this research, we proposed an explicit MGRIT method to solve a PDE equation by a parallel-in-time method with explicit schemes. We also tested the proposed method on one-dimensional heat transfer example and one-dimensional advection example. We show that the explicit MGRIT method works on both examples.

6. Future Work

Although the explicit MGRIT produces correct results and does not encounter the CFL condition trouble, since we do not apply direct solve at the coarsest layer, the iteration number grows with the problem size. This result does not necessarily mean that the speed is slow. The iteration number is still small, and we do not relax on the coarsest layer. How the speed performance is compared to the original MGRIT (with implicit schemes) is to be studied.

In this research, we have only tested the explicit MGRIT method on one dimensional PDE problems. For future work, we also hope to test the explicit MGRIT method on two or even three-dimensional examples. Only in this way can we fully explore the potential of this method.

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