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Parallelization Strategies for Ultrasonic Wave Propagation in Composite Materials Considering Microstructural Details

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This paper explores advanced parallelization strategies for simulating ultrasonic wave propagation in composite materials considering their complex microstructure. The grid-characteristic method and the use of Chimera grids in the simulations allow us to represent the composite material as an isotropic, linear-elastic medium and focus on improving the computational efficiency through efficient grid partitioning techniques. We used MPI (Message Passing Interface) technology on a high-performance computing cluster to test different methods for distributing computational grids across multiple processes. Our results highlight that partitioning grids according to material fiber layers improves the performance, especially when the number of processes matches the number of composite layers. This method not only provides better load balancing but also reduces communication overhead, making it the most efficient strategy tested. We present a comprehensive comparison of execution times and speedups for different partitioning approaches. Future work will aim to extend the study by increasing the number of layers and exploring how this approach scales with more complex and heterogeneous microstructures, potentially identifying further optimizations for parallel modeling.

Keywords: composite material, microstructure, grid characteristic method, parallelization.

Introduction

The accurate modeling of ultrasonic wave propagation in composite materials is essential for non-destructive evaluation (NDE) [4, 21], material testing, and structural health monitoring in industries such as aerospace [5, 12, 18], automotive [6, 22], and civil engineering [19, 23, 24]. Composite materials, due to their complex microstructures, require advanced computational approaches to capture the interactions between waves and internal structures, including fibers, voids, and other inclusions. These materials are typically heterogeneous, with varying elastic properties across different regions, making the wave propagation behavior significantly more complex compared to homogeneous materials.

Traditional numerical methods like the finite element method (FEM) and finite difference time domain (FDTD) are widely used in simulating ultrasonic waves in various materials [9, 10, 20]. However, when applied to composite materials, these methods often face limitations in terms of accuracy and computational efficiency, especially when high-frequency waves interact with fine microstructural features. The computational cost grows rapidly with the need to model small-scale features across large domains, particularly when simulating ultrasonic wave propagation at high frequencies or through intricate microstructures. Moreover, FEM and FDTD approaches often require complex meshing strategies, which can introduce errors and significantly increase computational overhead in handling boundary conditions between different material phases.

An alternative approach to simulating ultrasonic wave propagation in composite materials involves the use of anisotropic material models [2, 17, 25]. They are advantageous for representing the material's mechanical behavior with less need for complex meshing. However, their main drawback is the limited accuracy in handling intricate microstructural interactions, especially

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when fibers are oriented differently. High-precision methods like FEM offer better resolution for wave phenomena at fine scales, such as reflection and diffraction at material interfaces. Consequently, anisotropic models are less effective for simulations requiring detailed accuracy in complex microstructures.

To address these challenges, more advanced numerical techniques have been proposed, including the use of grid-characteristic methods (GCM) [15, 16] and Chimera grid approaches [8, 14], which have demonstrated significant potential in improving both the accuracy and scalability of wave propagation simulations in complex media [1, 3]. The grid-characteristic method provides a more natural way to handle wavefront propagation across material interfaces, allowing for higher accuracy in capturing reflection, refraction, and diffraction phenomena. By integrating Chimera grids, which allow the computational domain to be divided into overlapping subdomains with independent grids, it becomes possible to model composite materials with complex microstructures in a more efficient and flexible manner [13, 14].

Despite these advances, large-scale simulations of wave propagation in composite materials remain computationally demanding. The high-resolution grids required to accurately model the material's microstructure, coupled with the need for long simulation times to capture wave interactions, make these problems difficult to solve on single-node machines. For instance, when modeling ultrasonic wave propagation at high frequencies in a composite material with multiple layers or complex fiber orientations, the memory and computational power required can far exceed the capabilities of even high-end workstations. This is particularly true for non-destructive evaluation (NDE) and structural health monitoring applications, where high precision is required to detect flaws or defects within the material.

Given these challenges, parallel computing has come to the forefront to achieve acceleration of large-scale simulations. In particular, the use of distributed memory parallelization techniques, such as those enabled by Message Passing Interface (MPI), has become critical for solving these computationally intensive problems [7]. In our problem, it is possible to divide the computational grid between several processors, which allows scaling the simulation on high-performance computing (HPC) clusters. By distributing the computational load across multiple nodes, each with its own memory and computing unit, MPI enables high-resolution simulation of ultrasonic waves in problems with huge scale and many complex structures, such as composite materials.

In this study, we explored several grid parallelization approaches to achieve optimization in multilayer composite modeling. We have two types of computational grids describing both the fibers and the matrix within the composite, which can be partitioned in different ways for parallel processing. One common approach is uniform grid partitioning, where the domain is divided into equally sized subdomains. This approach is generally easy to implement, but may not be as efficient when applied to composites with highly heterogeneous microstructures. For example, uniform partitioning may result in some processors processing regions with complex fiber arrangements, while others process simpler regions, leading to load imbalances and ultimately reducing overall efficiency.

One of the most effective strategies, especially for multilayer composites, seems to be grid partitioning based on the natural structure of the material. This approach partitions the grid according to the arrangement of fibers in each layer, and this allows for a more even distribution of the computational load. In addition to evenly distributing the computational work, it is also important to minimize communication with other threads. This is especially effective when the

number of processes is a multiple of the number of layers, as it avoids sharing fibers from the same layer between different processes and minimizes the overhead of inter-process communication.

The performance of the uniform, layered-based, and hybrid partitioning strategies was evaluated using an HPC cluster. Each node in the cluster was equipped with dual-socket Intel Xeon processors and 256 GB of RAM. Performance metrics including execution time, speedup, and efficiency were measured as the number of processes varied. The results showed that the layer-based grid partitioning outperformed the uniform approach, especially as the number of processes increased.

By aligning the grid partitioning with the composite material structure, the layer-based approach achieved better load balancing and higher computational efficiency. A speedup analysis that compares the execution time with multiple processes to the execution time with a single process showed that the layer-based method provided improvements, especially when the number of processes was a multiple of the number of layers in the material. Of further interest is how the efficiency depends on the number of composite layers and the area of the material being modeled.

The paper is structured as follows. The Methods section describes our methods for modeling ultrasonic wave propagation, including the grid-characteristic approach and MPI-based parallelization. The Results section outlines the experimental setup and analyzes the results of different grid partitioning strategies. The conclusion and future directions are presented in the Conclusion section.

1. Methods

In this section, we provide a more detailed description of the methods used to model ultrasonic wave propagation in composite materials. The main focus is on the integration of the grid-characteristic method (GCM), Chimera grids, and parallelization techniques using MPI.

1.1. Grid-Characteristic Method (GCM)

In our study, the governing equations for wave propagation in linear elastic materials, such as fiber materials, form the system:

$$\rho\dot{\mathbf{v}} = (\nabla \cdot \boldsymbol{\sigma})^{\mathsf{T}}, \tag{1}$$

$$\dot{\boldsymbol{\sigma}} = \lambda (\nabla \cdot \mathbf{v}) \mathbf{I} + \mu (\nabla \otimes \mathbf{v} + (\nabla \otimes \mathbf{v})^{\mathsf{T}}), \tag{2}$$

where $\mathbf{v}$ is velocity vector, $\boldsymbol{\sigma}$ is Cauchy stress tensor and λ, μ are Lamé constants characterizing the properties of the material.

This is a system of first-order hyperbolic partial differential equations, which can be transformed to the folowing representation:

$$\frac{\partial \mathbf{u}}{\partial t} + A\frac{\partial \mathbf{u}}{\partial x} + B\frac{\partial \mathbf{u}}{\partial y} + C\frac{\partial \mathbf{u}}{\partial z} = 0, \tag{3}$$

where $\mathbf{u}$ represents the vector of unknowns (displacement and stress), and A, B, and C are coefficient matrices that depend on the material properties (e.g., density, elastic moduli).

GCM solves this system of equations by propagating information along the characteristic directions of the system using a structured grid that can be adapted to the geometry of the composite material. This approach is particularly effective in capturing wave reflections, transmissions, and interactions at interfaces between different materials within the composite.

In this work, free boundary conditions are applied at the outer boundaries of the computational domain. In addition, a no-slip condition is used to describe the interaction between the fibers and the surrounding matrix, simulating the physical adhesion between these components. These boundary conditions are conveniently taken into account by GCM, since the method handles such conditions naturally without the need for complex meshing or computational costs, preserving accuracy and simplifying the simulation setup.

1.2. Structured Curvilinear Grids

In fiber-reinforced composites, the fibers often have complex curved geometries. To accurately model the geometry and capture fine details of wave interactions, we use structured curvilinear grids. These grids allow us to represent the fibers and surrounding matrix with high accuracy without requiring excessive grid refinement in regions away from the interfaces.

To create curved grids, we map the physical domain of the composite material onto a reference domain using a transformation that preserves the geometric features of the fibers and matrix. This transformation is applied to the system of governing equations, yielding a modified set of equations that account for the curved nature of the grid. The coefficients of the transformed system are dynamically updated based on the Jacobian of the mapping at each grid point, as described in [8].

1.3. Chimera Grid Integration

One of the key innovations of our method is the integration of Chimera grids into the GCM framework. Chimera grids are overlapping grids that allow different regions of the composite material to be modeled independently at different grid resolutions. This is particularly useful when dealing with the heterogeneous nature of composite materials, where certain regions (e.g., near fibers) require finer grids, while other regions (e.g., in the matrix) can be modeled with coarser grids.

In our simulations, the background grid represents the global structure of the composite material, while individual Chimera grids are used to model individual fibers or other microstructural features at higher resolution. The Chimera grids are overlapped by the background grid, and the solution is interpolated between the grids at each time step.

Figure 1 illustrates the region of interest in the laminated composite material, where the computational grids were constructed. The background grid is shown in blue and the fibers are depicted in gray. The corresponding material parameters for this region are detailed in Tab. 1.

Table 1. Elasticity parameters of materials

Material	$c_p,\ m/s$	$c_s,\ m/s$	$\rho,\ kg/m^3$
Fiber	4003	3004	2000
Matrix	2553	1194	1160

Using Chimera grids allows us to focus computational resources on regions of interest, such as interfaces between materials, while maintaining the overall accuracy of the simulation.

Additionally, the independent nature of the Chimera grids lends itself well to parallelization, as the computations in each grid can be performed independently and then the results are interpolated back onto the background grid.

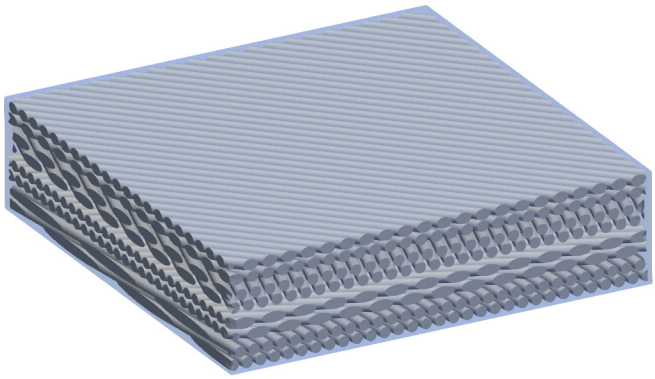


Figure 1. Representation of the structure of a composite material in the problem domain

1.4. Parallelization Using MPI

Given the complexity of the problem and the need for high-resolution simulations, parallelization is essential for achieving reasonable computation times. In our study, we employed MPI (Message Passing Interface) for the simmulation process parallelization across multiple processors in a distributed memory high-performance computing (HPC) cluster.

1.4.1. Parallelization strategy

Several parallelization strategies have been considered as a means of dividing the computational domain among several processes. These strategies include:

1. Uniform Grid Division (Fig. 2): In this approach, the computational grids are divided into uniform subdomains, with each subdomain assigned to a different process. This method is simple to implement but can lead to load imbalances, particularly in regions with complex microstructure, where some processes may have significantly more work than others.

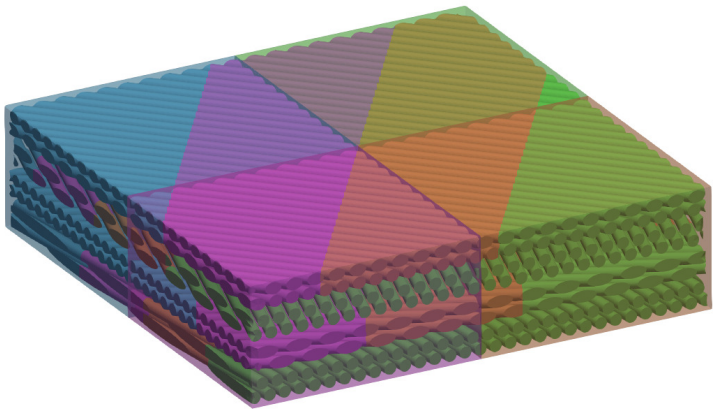


Figure 2. Uniform grid division (four colors correspond to four different processes)

2. Layer-Based Division (Fig. 3): Given the layered structure of many composite materials, we explored a parallelization strategy that divides the computational domain by layers. Each process is responsible for simulating one or more layers of the composite, with the number

of layers assigned to each process determined based on the total number of processes. This approach is particularly effective when the number of processes is a multiple of the number of layers, as it ensures a balanced distribution of the workload. The layer-based division strategy proved to be the most successful for our simulations. By aligning the computational grid division with the physical structure of the material (i.e., the location of fibers and matrix layers), we were able to achieve better load balancing and minimize communication overhead between processes.

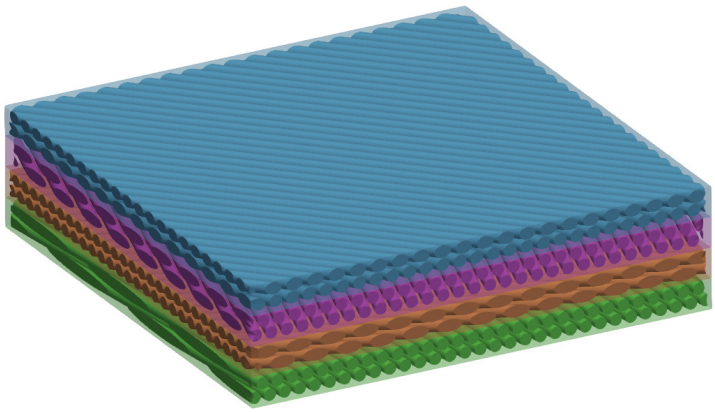


Figure 3. Layer-based division (four colors correspond to four different processes)

3. Hybrid Approach (Fig. 4): The idea here was to combine uniform grid partitioning and layer-based partitioning to achieve more flexible parallelization. For example, within each layer, the domain could be divided into smaller subdomains, which are then assigned to individual processes. This hybrid approach allowed us to gain a broader understanding of how each approach impacts the overall performance.

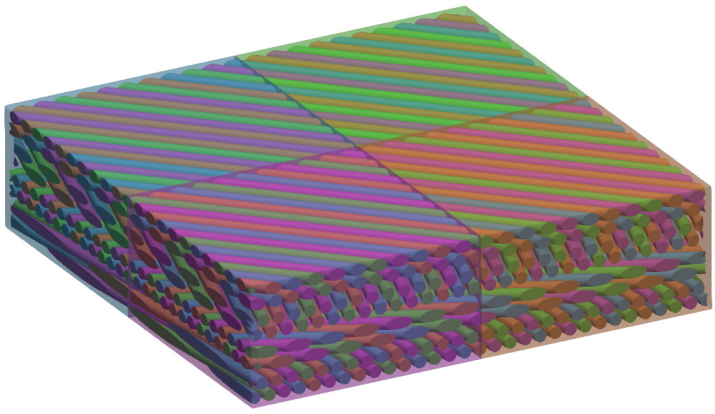


Figure 4. Hybrid approach division (four colors correspond to four different processes)

1.4.2. Communication and synchronization

MPI-based parallelization involves communication between processes to exchange information about the solution at the boundaries of each subdomain. In case of uniform grid division,

this communication occurs at the boundaries of each subdomain, where processes must exchange information about the displacement and stress fields. In the case of layer-based division, communication occurs between the processes responsible for adjacent layers.

To minimize the communication overhead, we implemented a non-blocking communication scheme using MPI's MPI_Isend and MPI_Irecv functions. This allows processes to continue computations while waiting for communication to complete, thereby reducing idle time and improving overall efficiency.

Synchronization between processes is required at each time step to ensure that the solution is consistent across the entire domain. This is particularly important when using Chimera grids, as the solution on each grid must be interpolated onto the background grid before proceeding to the next time step.

1.4.3. Performance metrics

To evaluate the performance of our parallelization strategies, we measured the execution time, speedup and efficiency for various configurations of processes and grid divisions. The speedup is defined as the ratio of the execution time on a single process to the execution time on multiple processes:

$$Speedup = \frac{T_1}{T_p},$$

where T_1 is the execution time on a single process, and T_p is the execution time on p processes. The efficiency is defined as follows:

$$Efficiency = \frac{Real\ Speedup}{Linear\ Speedup}.$$

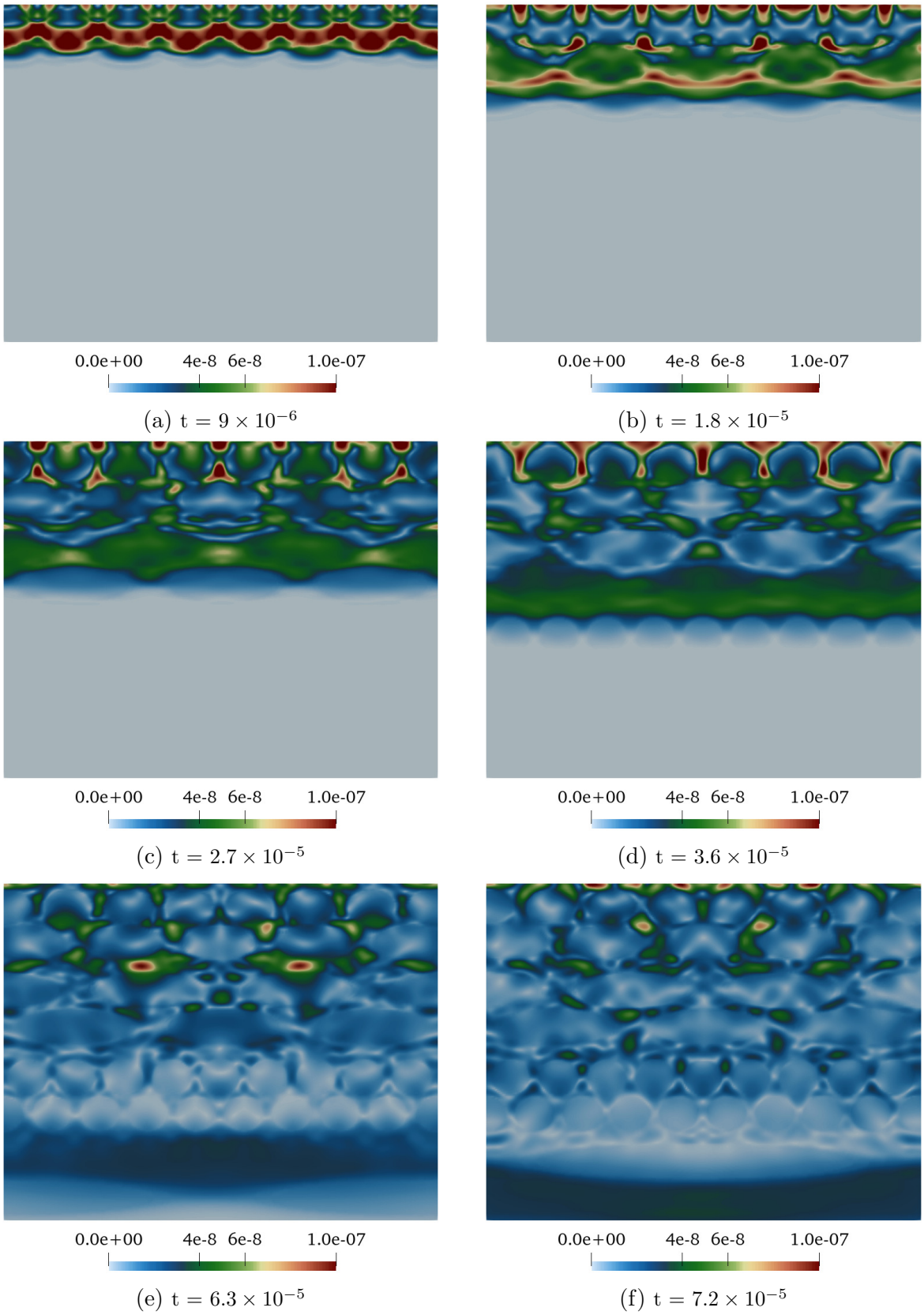
Our results, discussed in detail in the Results section, show that the layer-based division strategy provided the best performance, particularly when the number of processes was a multiple of the number of layers. This strategy also scaled well with increasing numbers of processes, achieving near-linear speedup in many cases.

2. Results

As a test case, we considered the problem of an elastic wave propagating through the cross-section of a composite material. A more detailed problem setup can be found in [13]. Solving this problem required approximately 50 GB of RAM due to the large number of computational grids, making the use of a cluster necessary. Figure 5 represents the speed field over the part of vertical cross-section of the composite material.

A comparison of execution time, speedup, and efficiency for different parallelization approaches with varying numbers of processes revealed similar results across methods (Fig. 6). However, the layer-based grid partitioning approach demonstrated better efficiency, particularly as the number of processes increased. Previous works on parallelizing composite grids for other types of problems showed less favorable results for the layer-based approach [11]. In contrast, the specific characteristics of our problem allowed us to achieve a significant performance improvement using this method.

It is important to note that parallelization in this context is particularly challenging, as the fibers, each assigned separate Chimera computational grids, are oriented in different directions.



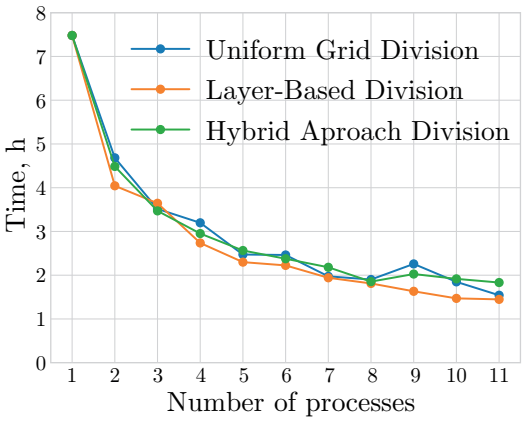
(a) t = 9×10^{-6} (b) t = 1.8×10^{-5}

(c) t = 2.7×10^{-5} (d) t = 3.6×10^{-5}

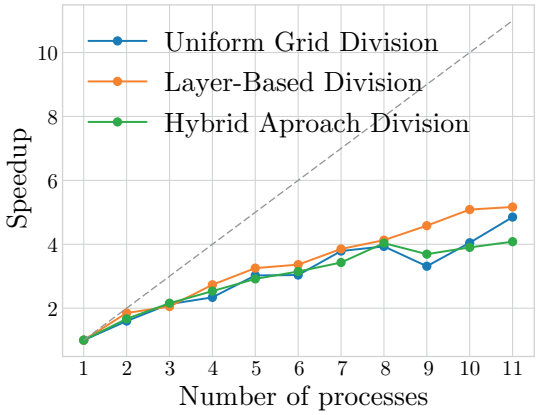
(e) t = 6.3×10^{-5} (f) t = 7.2×10^{-5}

Figure 5. Field ||**v**|| in the vertical section of composite at different moments of time t

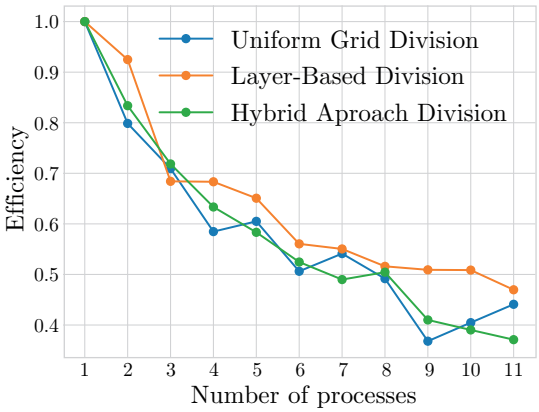
This orientation complexity makes it difficult to group closely related grid elements into a single process, further complicating the parallelization strategy.



(a) Execution time comparison



(b) Speedup metric comparison



(c) Efficiency metric comparison

Figure 6. Metrics for different approaches depending on the number of processes

Conclusion

This study presents a novel parallelization approach for simulating ultrasonic wave propagation in composite materials, specifically focusing on optimizing grid partitioning based on the materials microstructure. The layer-based division strategy, when aligned with the fiber layout of the composite, provides better performance, especially in cases where the number of processes matches the number of layers. Future work will focus on scaling these methods for more complex composites and exploring additional parallelization strategies.

By integrating the grid-characteristic method with MPI-based parallelization, we have laid the foundation for more efficient and accurate simulations, enabling better predictive capabilities for non-destructive testing and structural health monitoring in composite materials.

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