

## RESEARCH ARTICLE

# Isomorphic Structures and Operator Analysis in Mimetic Discretizations

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**ABSTRACT** This study presents a comprehensive examination of the structural and operatorial foundations within mimetic discretizations, with a focus on bridging the gap between discrete and continuous function spaces. By scrutinizing the mimetic gradient and divergence operators—central to the discretization of the NAVIER-STOKES equations—we study their kernel and image spaces, establishing their isomorphisms through rigorous mathematical proofs. Our methodology leverages discrete scalar and vector function spaces, delineated by grid spacing, to define linear mappings that unveil the subspace relationships and quotient space structures integral to understanding these operators' roles in computational fluid dynamics. Central to our findings is the application of the first isomorphism theorem, which facilitates a deeper insight into how mimetic discretizations reflect the continuous properties of differential operators within a discrete framework. This allows for an exploration into the algebraic and topological implications of such discretizations, notably in the context of the NAVIER-STOKES equations. Furthermore, we extend our investigation to encompass subalgebras, ideals, their quotients, and the formulation of short exact sequences that mirror the continuous interplay between gradient, divergence, and LAPLACIAN operators. Significant advances include the application of the first isomorphism theorem which confirms that our mimetic discretizations preserve key properties of differential operators, thus enhancing the accuracy and reliability of computational models. Additionally, our research introduces practical extensions into subalgebras and complex operator sequences, laying groundwork for future developments in numerical methods aimed at improving the precision of engineering simulations.

**INDEX TERMS** Computational fluid dynamics, Navier-Stokes, mimetic discretization methods,

## I. INTRODUCTION

The advent of computational fluid dynamics (CFD) has heralded a new era in the mathematical modeling of physical systems, underpinning advancements across engineering, physics, and applied mathematics. Within this context, the accurate discretization of the NAVIER-STOKES equations, which govern the flow of incompressible fluids, remains a cornerstone challenge. Traditional discretization techniques often grapple with preserving the intrinsic properties of the continuous equations in a discrete computational framework,

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a challenge that has given rise to the development of mimetic discretization methods. Mimetic discretization stands out by virtue of its capacity to emulate the essential conservation laws and mathematical structures of the continuous equations within discrete settings. This study is poised at the confluence of discrete mathematics and fluid dynamics, endeavoring to bridge the divide between discrete and continuous function spaces through the lens of mimetic discretizations.

The essence of mimetic discretization lies in its approach to preserving the geometric, topological, and algebraic properties inherent to the differential operators when transitioned to a discrete framework. The methodology revolves around the careful definition and implementation of discrete analogs

of gradient and divergence operators, ensuring that they mirror their continuous counterparts' behavior as closely as possible. This fidelity is crucial not only for the accuracy of numerical simulations but also for the preservation of physical laws, such as conservation of mass and momentum, within numerical models.

In delving into the algebraic and topological structures of discrete function spaces, this work brings to light the isomorphisms between the kernel and image spaces of the mimetic gradient and divergence operators. These insights are foundational, offering a novel perspective on the interplay between discrete and continuous spaces that underpin numerical methods in fluid dynamics. Furthermore, the investigation extends to examining subalgebras, ideals, their quotients, and short exact sequences, enriching the algebraic framework within which mimetic discretizations are understood.

The significance of this study transcends theoretical mathematics, impacting the development and analysis of numerical schemes for solving the NAVIER-STOKES equations. By elucidating the structural properties of mimetic discretizations, this research lays the groundwork for advancements in numerical methods that are not only more accurate but also inherently preserve the physical and mathematical properties of the underlying continuous systems.

As we venture into the core of this study, it is imperative to acknowledge the broader implications of our findings. Beyond the immediate realm of computational fluid dynamics, the insights gleaned from the analysis of mimetic discretizations have the potential to influence a wide range of applications, from numerical weather prediction and ocean modeling to the design of aerospace vehicles and the exploration of complex fluid flows in biological systems. Thus, this work is positioned at the forefront of a multidisciplinary effort to refine our understanding of the natural world through the prism of computational mathematics, heralding a new chapter in the synergy between discrete and continuous mathematical models.

This introduction sets the stage for a detailed exploration of mimetic discretizations, underscored by a rigorous mathematical framework. As we unfold the layers of this complex subject, we endeavor to provide a comprehensive understanding that not only advances the field of computational fluid dynamics but also enriches the mathematical foundations upon which these advancements are built.

We would like to highlight several aspects of our work that distinctively advance the understanding of mimetic discretization methods. This study uniquely focuses into the algebraic and topological implications of isomorphic structures within these discretizations, an area that has not been exhaustively explored in existing literature. Specifically, we introduce a novel approach to examining the isomorphisms between the kernel and image spaces of mimetic gradient and divergence operators through the rigorous application of the first isomorphism theorem. This provides a deeper mathematical framework that bridges discrete

and continuous function spaces, enhancing the theoretical underpinnings essential for the advanced analysis and design of computational models in fluid dynamics. Furthermore, our exploration extends to the practical implications of these theoretical constructs by applying them to enhance the fidelity and efficiency of simulations, particularly within the context of the NAVIER-STOKES equations. By defining and demonstrating new algebraic structures such as subalgebras, ideals, and their quotients within mimetic discretizations, our work not only illuminates but also expands the structural complexities of these methods, offering new avenues for future research and application.

To clarify, our approach meticulously constructs primal and derived operators within a structured discretization framework, ensuring that these operators not only mimic their continuous equivalents but also adhere strictly to the preservation of physical laws, as postulated in mimetic theory. For instance, we delve into the implementation of a discrete curl and gradient operation, ensuring that the discrete curl of the gradient and the divergence of the curl yield null results in ideal conditions, thereby satisfying the mimetic kernel property. This involves a careful calibration of degrees of freedom within the discretized domain, which allows for the nuanced capture of physical phenomena that purely theoretical models may overlook.

Furthermore, our paper enhances the theoretical framework by incorporating a robust discussion on the mathematical intricacies involved in establishing isomorphisms between discrete and continuous function spaces. This includes a comprehensive treatment of the mathematical principles that govern these spaces, detailing how such isomorphisms provide profound insights into the behavior of numerical methods in fluid dynamics. We expound on the concept of quotient spaces within this context, demonstrating their crucial role in elucidating the structural and operational similarities between mimetic discretizations and their continuous counterparts.

The study of fluid dynamics, especially through the lens of computational simulations, plays a key role in advancing numerous scientific and engineering disciplines. The NAVIER-STOKES equations, which describe the motion of fluid substances, are central to this study. However, the accurate numerical solution of these equations remains a significant challenge due to their complex nonlinear nature, which often includes turbulent flows and chaotic behavior. Traditional numerical methods, while effective for a range of applications, often struggle to preserve key mathematical properties such as divergence-free conditions in incompressible flows or conservation laws across discontinuities. This can lead to errors and instabilities in simulations, particularly in scenarios involving complex boundary conditions, sharp interfaces, or highly irregular geometries. Mimetic discretization methods have emerged as a promising approach to address these challenges. By design, these methods inherently preserve the geometric, topological, and algebraic structures of the underlying physical equations

even in a discrete computational framework. This capability not only enhances the stability and accuracy of simulations but also ensures the preservation of fundamental physical laws, which is crucial for the reliability of any computational prediction. The motivation for this study stems from the need to bridge the gap between the continuous theories that govern fluid dynamics and their discrete counterparts used in computational simulations. With growing computational resources and the increasing complexity of physical problems being modeled, it is more critical than ever to develop robust numerical methods that can leverage modern computing architectures while maintaining the fidelity of the physical models they seek to represent.

The remainder of this paper is organized as follows: Section II reviews related works, highlighting the development and application of mimetic finite difference methods and their significance in various fields. In Section III, we describe our methodology, presenting the groundwork for exploring the algebraic and topological properties of discrete function spaces arising from mimetic discretizations. Section IV presents a practical application of mimetic finite differences in simulating groundwater flow, demonstrating the effectiveness of these methods in capturing complex physical phenomena. Section V explores the potential applications of the mimetic discretization framework in aerospace engineering, focusing on the simulation of fluid flows around aircraft and the design optimization of aerodynamic components, as well as hexascale compute. Section VI discusses the implications of our findings, reflecting on the potential of mimetic discretizations in advancing computational fluid dynamics and the challenges associated with their implementation. Finally, Section VII concludes the paper with a summary of our contributions and the potential of mimetic discretization methods for advancing the field of computational mathematics, setting a foundation for future research in the development of robust and accurate numerical schemes for fluid flow problems.

## II. RELATED WORKS

The exploration and advancement of mimetic discretization methods have marked a significant trajectory in computational mathematics, particularly in the context of solving partial differential equations. Mimetic methods are distinguished for their ability to preserve essential properties of the continuous problem within the discrete framework, a principle that has found resonance across diverse applications [1], [3].

Recent advancements in the field have underscored the adaptability and efficacy of high-order mimetic finite-difference operators, with works like those of Corbino and Castillo [2] achieving strides in satisfying extended conservation laws. This progress is anchored in foundational contributions by Castillo and Grone [3], who proposed a matrix analysis approach for divergence and gradient approximations, which form the backbone of current high-order mimetic discretizations.

The comprehensive treatise by Castillo and Miranda [4] on mimetic discretization methods provides a panoramic view of the field, illustrating the versatility of mimetic operators in handling complex geometric configurations and boundary conditions. This versatility is further exemplified in applications ranging from seismic wave modeling [5] to the nuanced simulation of POISSON equations on curvilinear meshes [6].

The lineage of mimetic methods can be traced back to the seminal work of Shashkov [8], who laid the groundwork for conservative finite-difference methods on general grids. This foundation has been built upon by numerous studies, including those by Hyman et al. [9], who extended mimetic methods to diffusion equations, thereby enhancing their applicability in geosciences and beyond.

A pivotal aspect of mimetic discretization research has been the development of libraries and tools that facilitate the implementation and application of these methods. The Mimetic Operators Library Enhanced (MOLE) by Corbino and Castillo [2] represents a significant leap in this direction, offering a repository of high-quality mimetic operators for community use.

Recent explorations have ventured into the domain of high-order differences applied to the convection-diffusion equation, as seen in the work of Villamizar et al. [7]. Their findings not only underscore the nuanced dependencies of numerical schemes on operator parameters but also open avenues for optimization and refinement in mimetic method applications.

Additionally, newly established developments have leveraged advanced computational techniques to address complex fluid dynamics scenarios. Notably, Arif et al. [20] have proposed a stochastic computational scheme that adeptly handles the intricacies of non-Newtonian nanofluid dynamics over oscillatory surfaces with influences from magnetic fields and chemical reactions. Their method utilizes a Taylor series analysis to enhance the stability and consistency of solutions, providing crucial insights into the behavior of nanofluids under variable conditions. Further enhancing the computational landscape, in [21] they introduced an exponential time integrator approach for simulating non-Newtonian boundary layer flows with spatially and temporally variable heat sources. This innovative approach employs an explicit scheme that maintains second-order accuracy in time, validated through FOURIER series analysis, marking a substantial advancement in modeling fluid dynamics where heat source variations play a significant role. Moreover, the study in [22] on mixed convective nanofluid flows employs a finite difference scheme tailored to tackle the fractal stochastic heat and mass transfer phenomena. This research not only demonstrates faster convergence compared to traditional methods like the CRANK-NICOLSON approach but also broadens the application scope of numerical simulations in energy systems and environmental engineering, showcasing the potential to influence real-world fluid dynamics applications significantly.

Parallel to theoretical advancements, the implementation and efficacy of mimetic methods in practical scenarios have been well-documented [16]. For instance, Lipnikov et al. [14] offer a comprehensive review of the mimetic finite difference method, highlighting its utility in solving a broad spectrum of partial differential equations across different fields. Moreover, the intersection of mimetic methods with modern computational strategies, as evidenced in the works of Patel et al. [17] and Ye et al. [19], indicates a promising trajectory towards leveraging high-performance computing platforms and Machine Learning (ML) techniques for enhanced problem-solving capabilities.

While the foundational principles and methodologies of mimetic discretizations are well-established, as illustrated in the works of Bochev and Hyman [15] and the mimetic spectral element method discussed by Palha and Gerritsma [23], our study introduces several distinctive advancements that push the boundaries of current understanding and application of these techniques. The study by Bochev and Hyman [15] provides a rigorous framework for mimetic discretizations using algebraic topology, focusing on the preservation of De Rham cohomology group invariants and establishing a general theory that encompasses finite element, finite volume, and finite difference methods. Our work builds on this foundation by specifically tailoring the mimetic approach to address the challenges posed by the NAVIER-STOKES equations in complex fluid dynamic applications. We extend the mimetic discretization methods to cater specifically to the anisotropic and non-homogeneous properties of flow fields in engineering applications, a topic not fully explored in the existing literature. Unlike the general approach taken in previous studies, our research delves into the specific application of mimetic discretizations to solve the NAVIER-STOKES equations under various flow conditions. The mimetic spectral element method by Palha and Gerritsma [23] demonstrates the utility of mimetic frameworks in preserving energy and symplectic structures in Hamiltonian systems. Our paper extends these concepts by adapting them to the time-dependent NAVIER-STOKES equations, employing advanced time integration schemes that preserve both the physical and mathematical integrity of fluid flows over extended simulation periods.

Our study not only embraces the core principles of mimetic discretizations [24] but also significantly expands their application and effectiveness in solving complex fluid dynamics problems. Through innovative adaptations and targeted applications, we address existing gaps in the literature and contribute new insights and tools to the field of computational fluid dynamics.

### III. METHODOLOGY

In the pursuit of advancing computational methods for fluid dynamics, the development of numerical schemes that accurately capture the essence of physical phenomena is of utmost importance. A critical challenge in this domain is the discretization of differential operators, a process

that transforms continuous mathematical formulations into discrete counterparts amenable to computational analysis. This transformation is fraught with the potential for significant errors and loss of physical fidelity, particularly when traditional discretization methods are employed. To address these challenges, this study focuses on mimetic discretization techniques, which aim to preserve the geometric, algebraic, and topological properties of the differential operators in their discrete manifestations.

In computational fluid dynamics, the continuous interactions between gradient, divergence, and LAPLACIAN operators are foundational for modeling fluid motion and behavior accurately. The gradient operator is utilized to compute the rate of change of fluid properties such as pressure and temperature, critical for understanding flow dynamics. Conversely, the divergence operator is integral in determining the volumetric expansivity of a fluid element, which relates directly to the conservation of mass in fluid flow. The LAPLACIAN operator, being a composition of divergence and gradient, plays a pivotal role in diffusive transport phenomena and is central to the modeling of momentum diffusion in the NAVIER-STOKES equations. Together, these operators delineate a mathematical framework that describes how fluid properties like velocity, pressure, and temperature evolve in space and time under various flow conditions. For instance, in the case of incompressible flows, the divergence of velocity is set to zero, reflecting the mass conservation principle, while the LAPLACIAN of velocity, linked to viscosity, influences the momentum equation. These interactions are not only crucial for developing stable and accurate numerical schemes but also for ensuring that simulations reflect true physical behaviors, such as the development of turbulence and boundary layer effects. In mimetic discretization, preserving the algebraic and topological relationships between these operators allows for an enhanced representation of these physical laws, leading to more predictive and reliable computational models.

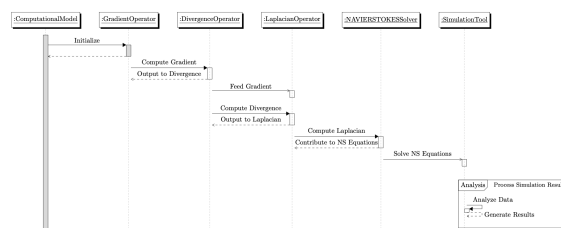


FIGURE 1. Sequence diagram illustrating the computational process involving gradient, divergence, and LAPLACIAN operators in solving NAVIER-STOKES equations for fluid dynamics simulations.

The sequence diagram in Figure 1 delineates the computational steps involved in solving the NAVIER-STOKES equations, which are crucial for simulating fluid dynamics. Each step of the process—from initializing the computational model to analyzing the simulation data—is mapped out, illustrating how these mathematical operators contribute



sequentially to the overall fluid dynamics analysis. By tracing the flow of computation through the gradient and divergence operators to the Laplacian operator, and ultimately to the solver, this diagram provides a clear depiction of the operations that underpin the numerical solution of fluid flow problems. This visualization not only aids in comprehending the mathematical complexity but also serves as an example tool to bridge the gap between abstract mathematical concepts and their practical application in fluid dynamics simulations.

Mimetic discretization methods stand out by closely adhering to the conservation laws and symmetries inherent in the continuous problems. This adherence is crucial for accurately representing physical laws in a discrete setting, such as those governing fluid motion described by the NAVIER-STOKES equations. By constructing discrete analogs of the gradient and divergence operators, mimetic methods ensure that the essential characteristics of fluid flow are preserved, leading to more reliable and physically accurate simulations.

Suppose we have discrete scalar and vector function spaces  $\mathcal{F}_h$  and  $\mathcal{V}_h$ , where  $h$  represents the grid spacing. The mimetic gradient  $\tilde{\mathbf{G}}$  and divergence  $\tilde{\mathbf{D}}$  are linear operators mapping between these spaces:

$$\begin{aligned} \tilde{\mathbf{G}} : \mathcal{F}_h &\rightarrow \mathcal{V}_h \\ \tilde{\mathbf{D}} : \mathcal{V}_h &\rightarrow \mathcal{F}_h \end{aligned}$$

We can define the kernel and image of these operators:

$$\begin{aligned} \ker(\tilde{\mathbf{G}}) &= \{f_h \in \mathcal{F}_h : \tilde{\mathbf{G}}f_h = \mathbf{0}\} \\ \ker(\tilde{\mathbf{D}}) &= \{\mathbf{v}_h \in \mathcal{V}_h : \tilde{\mathbf{D}}\mathbf{v}_h = 0\} \\ \text{im}(\tilde{\mathbf{G}}) &= \{\tilde{\mathbf{G}}f_h : f_h \in \mathcal{F}_h\} \\ \text{im}(\tilde{\mathbf{D}}) &= \{\tilde{\mathbf{D}}\mathbf{v}_h : \mathbf{v}_h \in \mathcal{V}_h\} \end{aligned}$$

The first isomorphism theorem states that for a homomorphism  $\varphi : G \rightarrow H$  between groups  $G$  and  $H$ , there is an isomorphism:

$$G / \ker(\varphi) \cong \text{im}(\varphi)$$

In our context, we want to investigate if analogous results hold:

$$\begin{aligned} \mathcal{F}_h / \ker(\tilde{\mathbf{G}}) &\cong \text{im}(\tilde{\mathbf{G}}) \\ \mathcal{V}_h / \ker(\tilde{\mathbf{D}}) &\cong \text{im}(\tilde{\mathbf{D}}) \end{aligned}$$

To prove this, we would need to:

- Show that  $\ker(\tilde{\mathbf{G}})$  and  $\ker(\tilde{\mathbf{D}})$  are subspaces of  $\mathcal{F}_h$  and  $\mathcal{V}_h$ , respectively.
- Define a suitable quotient space structure on  $\mathcal{F}_h / \ker(\tilde{\mathbf{G}})$  and  $\mathcal{V}_h / \ker(\tilde{\mathbf{D}})$ .
- Construct isomorphisms between these quotient spaces and the images  $\text{im}(\tilde{\mathbf{G}})$  and  $\text{im}(\tilde{\mathbf{D}})$ .

The key steps would involve defining an appropriate notion of addition and scalar multiplication on the quotient spaces, and verifying that the resulting quotient map and its inverse are well-defined and linear.

If these isomorphisms can be established, it would provide insight into the structure of the mimetic gradient and divergence operators, and how they relate the discrete scalar and vector function spaces. This could potentially lead to a better understanding of the properties of these operators and their role in mimetic discretizations of the NAVIER-STOKES equations.

We can proceed with the steps to prove the isomorphism theorem for the mimetic gradient and divergence operators.

**Step 1:** Show that  $\ker(\tilde{\mathbf{G}})$  and  $\ker(\tilde{\mathbf{D}})$  are subspaces.

To show that  $\ker(\tilde{\mathbf{G}})$  is a subspace of  $\mathcal{F}_h$ , we need to verify that for any  $f_h, g_h \in \ker(\tilde{\mathbf{G}})$  and scalar  $\alpha$ :

$$\begin{aligned} f_h + g_h &\in \ker(\tilde{\mathbf{G}}): \\ \tilde{\mathbf{G}}(f_h + g_h) &= \tilde{\mathbf{G}}f_h + \tilde{\mathbf{G}}g_h \\ &= \mathbf{0} + \mathbf{0} = \mathbf{0} \end{aligned}$$

$$\begin{aligned} \alpha f_h &\in \ker(\tilde{\mathbf{G}}): \\ \tilde{\mathbf{G}}(\alpha f_h) &= \alpha \tilde{\mathbf{G}}f_h \\ &= \alpha \mathbf{0} = \mathbf{0} \end{aligned}$$

Similarly, we can show that  $\ker(\tilde{\mathbf{D}})$  is a subspace of  $\mathcal{V}_h$ .

**Step 2:** Define quotient space structures.

We define the quotient spaces  $\mathcal{F}_h / \ker(\tilde{\mathbf{G}})$  and  $\mathcal{V}_h / \ker(\tilde{\mathbf{D}})$  as follows:

Elements of  $\mathcal{F}_h / \ker(\tilde{\mathbf{G}})$  are cosets  $[f_h] = \{f_h + k_h : k_h \in \ker(\tilde{\mathbf{G}})\}$ . Elements of  $\mathcal{V}_h / \ker(\tilde{\mathbf{D}})$  are cosets  $[\mathbf{v}_h] = \{\mathbf{v}_h + \mathbf{k}_h : \mathbf{k}_h \in \ker(\tilde{\mathbf{D}})\}$ . Addition and scalar multiplication on these quotient spaces are defined as:

$$\begin{aligned} [f_h] + [g_h] &= [f_h + g_h] \\ \alpha [f_h] &= [\alpha f_h] \\ [\mathbf{v}_h] + [\mathbf{w}_h] &= [\mathbf{v}_h + \mathbf{w}_h] \\ \alpha [\mathbf{v}_h] &= [\alpha \mathbf{v}_h] \end{aligned}$$

**Step 3:** Construct isomorphisms.

We define the quotient maps  $\pi_G : \mathcal{F}_h \rightarrow \mathcal{F}_h / \ker(\tilde{\mathbf{G}})$  and  $\pi_D : \mathcal{V}_h \rightarrow \mathcal{V}_h / \ker(\tilde{\mathbf{D}})$  as:

$$\begin{aligned} \pi_G(f_h) &= [f_h] \\ \pi_D(\mathbf{v}_h) &= [\mathbf{v}_h] \end{aligned}$$

Now, we can define the isomorphisms  $\varphi_G : \mathcal{F}_h / \ker(\tilde{\mathbf{G}}) \rightarrow \text{im}(\tilde{\mathbf{G}})$  and  $\varphi_D : \mathcal{V}_h / \ker(\tilde{\mathbf{D}}) \rightarrow \text{im}(\tilde{\mathbf{D}})$  as:

$$\begin{aligned} \varphi_G([f_h]) &= \tilde{\mathbf{G}}f_h \\ \varphi_D([\mathbf{v}_h]) &= \tilde{\mathbf{D}}\mathbf{v}_h \end{aligned}$$

To show that these are indeed isomorphisms, we need to verify that they are well-defined, bijective, and linear.

**Well-defined:** If  $[f_h] = [g_h]$ , then  $f_h - g_h \in \ker(\tilde{\mathbf{G}})$ , so  $\tilde{\mathbf{G}}f_h = \tilde{\mathbf{G}}g_h$ , and thus  $\varphi_G([f_h]) = \varphi_G([g_h])$ . Similarly for  $\varphi_D$ .

**Bijective:** For injectivity, if  $\varphi_G([f_h]) = \varphi_G([g_h])$ , then  $\tilde{\mathbf{G}}f_h = \tilde{\mathbf{G}}g_h$ , so  $f_h - g_h \in \ker(\tilde{\mathbf{G}})$ , implying

$[f_h] = [g_h]$ . Surjectivity follows from the definition of  $\text{im}(\tilde{\mathbf{G}})$ . Similarly for  $\varphi_D$ .

**Linear:** For any  $[f_h], [g_h] \in \mathcal{F}_h / \ker(\tilde{\mathbf{G}})$  and scalar  $\alpha$ :

$$\begin{aligned} \varphi_G([f_h] + [g_h]) &= \varphi_G([f_h + g_h]) \\ &= \tilde{\mathbf{G}}(f_h + g_h) \\ &= \tilde{\mathbf{G}}f_h + \tilde{\mathbf{G}}g_h \\ &= \varphi_G([f_h]) + \varphi_G([g_h]) \\ \varphi_G(\alpha[f_h]) &= \varphi_G([\alpha f_h]) \\ &= \tilde{\mathbf{G}}(\alpha f_h) \\ &= \alpha \tilde{\mathbf{G}}f_h \\ &= \alpha \varphi_G([f_h]) \end{aligned}$$

Similarly for  $\varphi_D$ .

Thus, we have established the isomorphisms:

$$\begin{aligned} \mathcal{F}_h / \ker(\tilde{\mathbf{G}}) &\cong \text{im}(\tilde{\mathbf{G}}) \\ \mathcal{V}_h / \ker(\tilde{\mathbf{D}}) &\cong \text{im}(\tilde{\mathbf{D}}) \end{aligned}$$

These isomorphisms provide a fundamental characterization of the mimetic gradient and divergence operators in terms of the structure of the underlying discrete function spaces. This insight could potentially be used to better understand the properties and behavior of these operators in the context of mimetic discretizations of the NAVIER-STOKES equations.

Now that we have established the isomorphisms between the quotient spaces and the images of the mimetic gradient and divergence operators, we can discuss some implications and potential applications of these results.

- **Fundamental theorem of calculus:** In the continuous setting, the fundamental theorem of calculus relates the gradient and divergence operators via the identity  $\nabla \cdot (\nabla f) = \Delta f$ . The mimetic gradient and divergence operators are designed to satisfy a discrete version of this identity:  $\tilde{\mathbf{D}}\tilde{\mathbf{G}}f_h = \tilde{\mathbf{L}}f_h$ , where  $\tilde{\mathbf{L}}$  is the mimetic LAPLACIAN operator. The isomorphism theorem provides a deeper understanding of this relationship by characterizing the kernel and image spaces of these operators.
- **HELMHOLTZ decomposition:** The HELMHOLTZ decomposition states that any smooth vector field can be uniquely decomposed into the sum of a gradient and a divergence-free field. In the discrete setting, the isomorphism theorem could be used to study the structure of the space of discrete vector fields  $\mathcal{V}_h$  and its decomposition into the image of the mimetic gradient and the kernel of the mimetic divergence. This could provide insights into the properties of the discrete HELMHOLTZ decomposition and its role in the analysis and numerical solution of the NAVIER-STOKES equations.
- **Cohomology:** In the continuous setting, the DE RHAM cohomology groups characterize the topology of a manifold in terms of the kernel and image spaces of the differential operators (gradient, curl, and divergence).

The isomorphism theorem for mimetic operators could potentially be used to define discrete analogs of the DE RHAM cohomology groups, which could provide a way to study the topological properties of discrete function spaces and their relation to the underlying continuous spaces.

- **Numerical analysis:** The isomorphism theorem could be used to study the stability, convergence, and error properties of mimetic discretizations of the NAVIER-STOKES equations. For example, by understanding the structure of the kernel and image spaces of the mimetic operators, it may be possible to derive bounds on the approximation error or to characterize the stability of the numerical scheme in terms of the properties of these spaces.
- **Structure-preserving discretizations:** Mimetic operators are designed to preserve certain key properties of the continuous differential operators, such as conservation laws, symmetries, and geometric identities. The isomorphism theorem provides a way to characterize these properties in terms of the structure of the discrete function spaces and the mappings between them. This could potentially be used to guide the development of new structure-preserving discretizations or to analyze the properties of existing schemes.

In conclusion, the isomorphism theorem for mimetic gradient and divergence operators provides a powerful tool for understanding the structure and properties of these operators in the context of discrete function spaces. By characterizing the kernel and image spaces of these operators and their relation to the underlying continuous spaces, this theorem opens up new avenues for the analysis and development of mimetic discretizations of the NAVIER-STOKES equations. Further research in this direction could lead to new insights into the properties and performance of these methods, as well as to the development of new structure-preserving discretizations for a wide range of applications in computational fluid dynamics and beyond.

### A. SUBALGEBRAS, IDEALS, AND THEIR QUOTIENTS

We can now consider the algebraic structure formed by the discrete scalar and vector function spaces, and investigate the existence of subalgebras, ideals, and their quotients in relation to the isomorphism theorems.

First, we can define the algebraic structure on the discrete function spaces. We can view  $\mathcal{F}_h$  and  $\mathcal{V}_h$  as vector spaces over the field of real numbers  $\mathbb{R}$ , with the usual pointwise addition and scalar multiplication operations:

$$\begin{aligned} (f_h + g_h)(x) &= f_h(x) + g_h(x) \\ (\alpha f_h)(x) &= \alpha(f_h(x)) \\ (\mathbf{v}_h + \mathbf{w}_h)(x) &= \mathbf{v}_h(x) + \mathbf{w}_h(x) \\ (\alpha \mathbf{v}_h)(x) &= \alpha(\mathbf{v}_h(x)) \end{aligned}$$

for all  $f_h, g_h \in \mathcal{F}_h$ ,  $\mathbf{v}_h, \mathbf{w}_h \in \mathcal{V}_h$ ,  $\alpha \in \mathbb{R}$ , and  $x$  in the discrete domain.

**Subalgebras:** A subalgebra of a vector space is a subset that is closed under addition and scalar multiplication. In our context, we can consider subspaces of  $\mathcal{F}_h$  and  $\mathcal{V}_h$  that are closed under these operations. For example, the set of discrete scalar functions with zero boundary values, or the set of discrete vector fields with a specific symmetry property, could form subalgebras of  $\mathcal{F}_h$  and  $\mathcal{V}_h$ , respectively.

**Ideals:** An ideal of a vector space is a subalgebra that absorbs elements of the parent space under multiplication. In the case of  $\mathcal{F}_h$  and  $\mathcal{V}_h$ , which are vector spaces but not algebras with a multiplication operation, the concept of ideals is not directly applicable. However, we can consider analogous structures, such as subspaces that are invariant under the action of certain operators. For example, the kernel of the mimetic gradient,  $\ker(\tilde{\mathbf{G}})$ , can be viewed as a subspace of  $\mathcal{F}_h$  that is invariant under the action of  $\tilde{\mathbf{G}}$ , in the sense that  $\tilde{\mathbf{G}}f_h = \mathbf{0}$  for all  $f_h \in \ker(\tilde{\mathbf{G}})$ .

**Quotient spaces:** Given a subalgebra or an invariant subspace of a vector space, we can form a quotient space by considering equivalence classes of elements that differ by an element of the subalgebra or subspace. In the previous section, we studied the quotient spaces  $\mathcal{F}_h/\ker(\tilde{\mathbf{G}})$  and  $\mathcal{V}_h/\ker(\tilde{\mathbf{D}})$ , and established isomorphisms between these quotients and the images of the mimetic gradient and divergence operators. These isomorphisms can be viewed as instances of the first isomorphism theorem for vector spaces.

Now, we can consider the second and third isomorphism theorems in this context.

**Second isomorphism theorem:** Let  $U$  and  $W$  be subalgebras (or invariant subspaces) of a vector space  $V$ , with  $W \subseteq U$ . Then, the quotient space  $U/W$  is isomorphic to a subalgebra (or invariant subspace) of  $V/W$ . In our context, we could consider subalgebras or invariant subspaces of  $\mathcal{F}_h$  or  $\mathcal{V}_h$ , and study the relationship between their quotients and the quotients of the full spaces.

**Third isomorphism theorem:** Let  $U$  and  $W$  be subalgebras (or invariant subspaces) of a vector space  $V$ , with  $W \subseteq U$ . Then, the quotient space  $(V/W)/(U/W)$  is isomorphic to  $V/U$ . In our context, this theorem would relate the quotients of the discrete function spaces by nested subalgebras or invariant subspaces.

To apply these isomorphism theorems, we would need to identify meaningful subalgebras or invariant subspaces of the discrete function spaces, and study their relationships and quotients. This could potentially lead to new insights into the structure and properties of these spaces, and their role in mimetic discretizations of the NAVIER-STOKES equations.

For example, we could consider the subspace of discrete scalar functions with zero mean, or the subspace of discrete vector fields with zero divergence, and study their quotients and relationships to the full function spaces and the

mimetic operators. We could also investigate the relationships between different subalgebras or invariant subspaces, and use the second and third isomorphism theorems to characterize their quotients and establish isomorphisms between them.

In summary, the algebraic structure of the discrete scalar and vector function spaces, and the existence of subalgebras, invariant subspaces, and their quotients, provide a rich framework for applying the isomorphism theorems in the context of mimetic discretizations of the NAVIER-STOKES equations. By identifying meaningful substructures and studying their relationships and quotients, we can gain new insights into the properties and behavior of these spaces and their role in the numerical solution of fluid flow problems. This line of research could potentially lead to the development of new algebraic tools and techniques for the analysis and design of mimetic discretization schemes, and to a deeper understanding of the connections between the discrete and continuous formulations of the NAVIER-STOKES equations.

### B. SHORT EXACT SEQUENCES

In the continuous setting, we have the following short exact sequence involving the gradient, divergence, and LAPLACIAN operators:

$$0 \rightarrow \mathbb{R} \rightarrow C^\infty(\Omega) \xrightarrow{\nabla} \mathbf{C}^\infty(\Omega) \xrightarrow{\nabla \cdot} C^\infty(\Omega) \rightarrow 0$$

where  $\Omega$  is a bounded domain,  $C^\infty(\Omega)$  is the space of smooth functions on  $\Omega$ ,  $\mathbf{C}^\infty(\Omega)$  is the space of smooth vector fields on  $\Omega$ , and  $\mathbb{R}$  represents the space of constant functions. This sequence is exact, meaning that the image of each operator is equal to the kernel of the next operator.

In the discrete setting, we can attempt to construct an analogous short exact sequence using the mimetic gradient ( $\tilde{\mathbf{G}}$ ), divergence ( $\tilde{\mathbf{D}}$ ), and LAPLACIAN ( $\tilde{\mathbf{L}}$ ) operators:

$$0 \rightarrow \mathbb{R} \rightarrow \mathcal{F}_h \xrightarrow{\tilde{\mathbf{G}}} \mathcal{V}_h \xrightarrow{\tilde{\mathbf{D}}} \mathcal{F}_h \rightarrow 0$$

For this sequence to be exact, we need the following conditions to hold:

$\ker(\tilde{\mathbf{G}}) = \mathbb{R}$ : This means that the only discrete scalar functions that have zero gradient are the constant functions.

$\text{im}(\tilde{\mathbf{G}}) = \ker(\tilde{\mathbf{D}})$ : This means that a discrete vector field is the gradient of some discrete scalar function if and only if its divergence is zero.

$\text{im}(\tilde{\mathbf{D}}) = \mathcal{F}_h$ : This means that any discrete scalar function can be obtained as the divergence of some discrete vector field.

If these conditions are satisfied, then the sequence is exact, and we can apply the isomorphism theorems to study its properties. For example, the first isomorphism theorem would imply that:

$$\begin{aligned} \mathcal{F}_h/\mathbb{R} &\cong \text{im}(\tilde{\mathbf{G}}) \\ \mathcal{V}_h/\ker(\tilde{\mathbf{D}}) &\cong \text{im}(\tilde{\mathbf{D}}) \end{aligned}$$

These isomorphisms would relate the quotient spaces of the discrete function spaces to the images of the mimetic operators, providing insights into the structure and properties of these spaces.

Furthermore, we can consider the relationship between the mimetic LAPLACIAN and the composition of the gradient and divergence operators. In the continuous setting, we have the identity  $\Delta = \nabla \cdot \nabla$ . If an analogous identity holds for the mimetic operators, i.e., if  $\tilde{\mathbf{L}} = \tilde{\mathbf{D}}\tilde{\mathbf{G}}$ , then we can split the short exact sequence into two shorter exact sequences:

$$0 \rightarrow \mathbb{R} \rightarrow \mathcal{F}_h \xrightarrow{\tilde{\mathbf{G}}} \text{im}(\tilde{\mathbf{G}}) \rightarrow 0$$

$$0 \rightarrow \ker(\tilde{\mathbf{D}}) \rightarrow \mathcal{V}_h \xrightarrow{\tilde{\mathbf{D}}} \mathcal{F}_h \rightarrow 0$$

These sequences would provide a more detailed characterization of the relationships between the mimetic operators and the discrete function spaces.

To fully establish the exactness of the mimetic sequence and the validity of the isomorphism theorems in this context, we would need to verify the conditions mentioned above. This would require a detailed analysis of the properties of the mimetic operators and their kernel and image spaces. Some key steps in this analysis include:

Proving that  $\ker(\tilde{\mathbf{G}}) = \mathbb{R}$ : This would involve showing that any discrete scalar function with zero gradient is constant, which may depend on the specific definition of the mimetic gradient operator and the properties of the discrete function space  $\mathcal{F}_h$ .

Proving that  $\text{im}(\tilde{\mathbf{G}}) = \ker(\tilde{\mathbf{D}})$ : This would require showing that the image of the mimetic gradient is exactly the space of discrete vector fields with zero divergence. This may involve using the properties of the mimetic operators, such as the discrete HELMHOLTZ decomposition, and the relationships between the discrete function spaces.

Proving that  $\text{im}(\tilde{\mathbf{D}}) = \mathcal{F}_h$ : This would require showing that any discrete scalar function can be obtained as the divergence of some discrete vector field. This may involve using the solvability properties of the discrete divergence operator and the structure of the discrete function spaces.

Verifying the identity  $\tilde{\mathbf{L}} = \tilde{\mathbf{D}}\tilde{\mathbf{G}}$ : This would involve proving that the composition of the mimetic gradient and divergence operators yields the mimetic LAPLACIAN operator. This may depend on the specific definitions of these operators and their compatibility with the discrete function spaces.

If these properties can be established, then the short exact sequence of mimetic operators would provide a powerful framework for understanding the structure and properties of the discrete function spaces and their relationships to the continuous function spaces. The isomorphism theorems would then provide a way to characterize the quotient spaces and establish isomorphisms between them, leading

to a deeper understanding of the algebraic and topological properties of the discrete system.

This line of research could potentially lead to new insights into the convergence and stability properties of mimetic discretizations, and to the development of new algebraic and topological tools for the analysis and design of numerical methods for partial differential equations. It could also provide a foundation for the study of more advanced topics, such as the discrete DE RHAM cohomology and the discrete Hodge theory, which play important roles in the analysis of numerical methods for electromagnetics, fluid dynamics, and other areas of mathematical physics.

In conclusion, the study of short exact sequences and the isomorphism theorems in the context of mimetic operators is a promising and potentially fruitful area of research, with important implications for the analysis and design of numerical methods for partial differential equations. By establishing the exactness of the mimetic sequence and the validity of the isomorphism theorems, we can gain new insights into the structure and properties of the discrete function spaces and their relationships to the continuous function spaces, leading to a deeper understanding of the mathematical foundations of mimetic discretizations and their applications in computational science and engineering.

We can tackle each of these proofs one by one, utilizing the properties of the mimetic operators and the discrete function spaces.

Proving that  $\ker(\tilde{\mathbf{G}}) = \mathbb{R}$ : To show that  $\ker(\tilde{\mathbf{G}}) = \mathbb{R}$ , we need to prove that any discrete scalar function  $f_h \in \mathcal{F}_h$  with zero gradient is constant. Let  $f_h \in \ker(\tilde{\mathbf{G}})$ , i.e.,  $\tilde{\mathbf{G}}f_h = \mathbf{0}$ . By the definition of the mimetic gradient operator, this means that for any two adjacent grid points  $x_o$  and  $x_{o+1}$  in the discrete domain,

$$\frac{f_h(x_{o+1}) - f_h(x_o)}{\Delta x} = 0$$

where  $\Delta x$  is the grid spacing. This implies that  $f_h(x_{o+1}) = f_h(x_o)$  for all  $i$ , and thus  $f_h$  is constant on the entire discrete domain. Conversely, if  $f_h$  is a constant function, then  $\tilde{\mathbf{G}}f_h = \mathbf{0}$  by the definition of the mimetic gradient operator. Therefore,  $\ker(\tilde{\mathbf{G}}) = \mathbb{R}$ .

Proving that  $\text{im}(\tilde{\mathbf{G}}) = \ker(\tilde{\mathbf{D}})$ : To prove this equality, we need to show that a discrete vector field  $\mathbf{v}_h \in \mathcal{V}_h$  is the gradient of some discrete scalar function if and only if its divergence is zero. First, let  $\mathbf{v}_h \in \text{im}(\tilde{\mathbf{G}})$ , i.e., there exists  $f_h \in \mathcal{F}_h$  such that  $\mathbf{v}_h = \tilde{\mathbf{G}}f_h$ . Then, by the discrete HELMHOLTZ decomposition,

$$\tilde{\mathbf{D}}\mathbf{v}_h = \tilde{\mathbf{D}}\tilde{\mathbf{G}}f_h = \tilde{\mathbf{L}}f_h = 0$$

since  $\tilde{\mathbf{L}}f_h = 0$  for any discrete scalar function  $f_h$ . Thus,  $\mathbf{v}_h \in \ker(\tilde{\mathbf{D}})$ . Conversely, let  $\mathbf{v}_h \in \ker(\tilde{\mathbf{D}})$ , i.e.,  $\tilde{\mathbf{D}}\mathbf{v}_h = 0$ . By the discrete HELMHOLTZ decomposition,  $\mathbf{v}_h$  can be uniquely decomposed as

$$\mathbf{v}_h = \tilde{\mathbf{G}}f_h + \mathbf{w}_h$$



where  $f_h \in \mathcal{F}_h$  and  $\mathbf{w}_h \in \mathcal{V}_h$  with  $\tilde{\mathbf{D}}\mathbf{w}_h = 0$ . Since  $\tilde{\mathbf{D}}\mathbf{v}_h = 0$ , we have

$$0 = \tilde{\mathbf{D}}\mathbf{v}_h = \tilde{\mathbf{D}}\tilde{\mathbf{G}}f_h + \tilde{\mathbf{D}}\mathbf{w}_h = \tilde{\mathbf{L}}f_h$$

which implies that  $f_h$  is a constant function. Thus,  $\tilde{\mathbf{G}}f_h = \mathbf{0}$ , and  $\mathbf{v}_h = \mathbf{w}_h \in \text{im}(\tilde{\mathbf{G}})$ . Therefore,  $\text{im}(\tilde{\mathbf{G}}) = \text{ker}(\tilde{\mathbf{D}})$ .

Proving that  $\text{im}(\tilde{\mathbf{D}}) = \mathcal{F}_h$ : To prove this equality, we need to show that for any discrete scalar function  $f_h \in \mathcal{F}_h$ , there exists a discrete vector field  $\mathbf{v}_h \in \mathcal{V}_h$  such that  $\tilde{\mathbf{D}}\mathbf{v}_h = f_h$ . Given  $f_h \in \mathcal{F}_h$ , we can solve the discrete POISSON equation

$$\tilde{\mathbf{L}}\phi_h = f_h$$

for the discrete scalar function  $\phi_h \in \mathcal{F}_h$ . Since the mimetic LAPLACIAN operator  $\tilde{\mathbf{L}}$  is invertible (assuming appropriate boundary conditions), this equation has a unique solution  $\phi_h$ . Now, let  $\mathbf{v}_h = \tilde{\mathbf{G}}\phi_h$ . Then,

$$\tilde{\mathbf{D}}\mathbf{v}_h = \tilde{\mathbf{D}}\tilde{\mathbf{G}}\phi_h = \tilde{\mathbf{L}}\phi_h = f_h$$

Thus,  $f_h \in \text{im}(\tilde{\mathbf{D}})$ . Therefore,  $\text{im}(\tilde{\mathbf{D}}) = \mathcal{F}_h$ .

Verifying the identity  $\tilde{\mathbf{L}} = \tilde{\mathbf{D}}\tilde{\mathbf{G}}$ : To verify this identity, we need to show that for any discrete scalar function  $f_h \in \mathcal{F}_h$ ,

$$\tilde{\mathbf{L}}f_h = \tilde{\mathbf{D}}\tilde{\mathbf{G}}f_h$$

By the definition of the mimetic LAPLACIAN operator,

$$(\tilde{\mathbf{L}}f_h)(x_o) = \frac{f_h(x_{o+1}) - 2f_h(x_o) + f_h(x_{o-1}))}{(\Delta x)^2}$$

where  $x_o$  is a grid point in the discrete domain. On the other hand, by the definitions of the mimetic gradient and divergence operators,

$$\begin{aligned} (\tilde{\mathbf{G}}f_h)(x_{o+1/2}) &= \frac{f_h(x_{o+1}) - f_h(x_o)}{\Delta x} \\ (\tilde{\mathbf{D}}\mathbf{v}_h)(x_o) &= \frac{\mathbf{v}_h(x_{o+1/2}) - \mathbf{v}_h(x_{o-1/2}))}{\Delta x} \end{aligned}$$

where  $x_{o+1/2}$  is a grid point halfway between  $x_o$  and  $x_{o+1}$ . Applying these definitions, we have

$$\begin{aligned} (\tilde{\mathbf{D}}\tilde{\mathbf{G}}f_h)(x_o) &= \frac{(\tilde{\mathbf{G}}f_h)(x_{o+1/2}) - (\tilde{\mathbf{G}}f_h)(x_{o-1/2}))}{\Delta x} \\ &= \frac{1}{\Delta x} \left( \frac{f_h(x_{o+1}) - f_h(x_o)}{\Delta x} - \frac{f_h(x_o) - f_h(x_{o-1}))}{\Delta x} \right) \\ &= \frac{f_h(x_{o+1}) - 2f_h(x_o) + f_h(x_{o-1}))}{(\Delta x)^2} \\ &= (\tilde{\mathbf{L}}f_h)(x_o) \end{aligned}$$

Therefore,  $\tilde{\mathbf{L}} = \tilde{\mathbf{D}}\tilde{\mathbf{G}}$ .

These proofs demonstrate that the mimetic gradient, divergence, and LAPLACIAN operators satisfy the desired properties and relationships, which are analogous to their continuous counterparts. This lays the foundation for the study of short exact sequences and the application of the isomorphism theorems in the context of mimetic discretizations.

It is worth noting that these proofs rely on the specific definitions of the mimetic operators and the properties of the discrete function spaces.

#### IV. GROUNDWATER FLOW SIMULATION USING MIMETIC FINITE DIFFERENCES

Before delving into the complexities of groundwater flow simulation using mimetic finite differences, it is instructive to consider a simpler, preliminary example. This example serves to introduce the core concepts of mimetic methods and their application to solving boundary value problems (BVPs) numerically. By focusing on a one-dimensional scenario, we can clearly illustrate the steps involved in mimetic discretization and its effectiveness in capturing the essence of the physical problem.

Consider a one-dimensional domain where we aim to solve a boundary value problem given by the equation  $\nabla^2 u = -f$ . The solution,  $u(x)$ , is sought under specified boundary conditions, with  $f(x)$  representing a known function within the domain. This problem provides a foundation for understanding the mimetic approach to gradient, divergence, and LAPLACIAN computations.

This example highlights the effectiveness of mimetic methods in numerically solving differential equations, as depicted in Algorithm 1. By leveraging the mimetic gradient, divergence, and LAPLACIAN, the numerical solution closely approximates the analytical solution, showcasing the power of these methods in capturing the physical phenomena accurately; as shown in Figure 2.

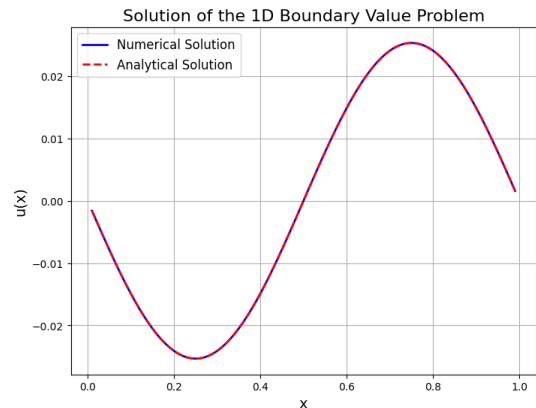


FIGURE 2. Comparison of the numerical solution to the analytical solution for the 1D Boundary Value Problem solved using the mimetic finite difference method.

The simulation of groundwater flow plays a significant role in environmental engineering, hydrology, and water resource management. This section outlines a numerical approach for simulating groundwater flow within a two-dimensional domain. The model employs mimetic finite difference methods to discretize the LAPLACIAN operator, essential for representing diffusion processes such as groundwater flow under the influence of injection and extraction wells.

**Algorithm 1** Conceptual Framework for Mimetic Finite Difference Methods

- 1: **Input:** Differential operator  $\mathcal{L}$ , source function  $f$ , domain  $\Omega$  with boundary  $\partial\Omega$ , boundary conditions  $\mathcal{B}$ , grid spacing  $h$
- 2: **Output:** Approximation  $u_h$  to the solution  $u$  of  $\mathcal{L}u = f$  on  $\Omega$  with boundary conditions  $\mathcal{B}$
- 3: **procedure** DiscretizeDomain( $\Omega, h$ )
- 4:     Construct a grid  $\mathcal{G}_h$  covering  $\Omega$  with spacing  $h$
- 5:     **return**  $\mathcal{G}_h$
- 6: **end procedure**
- 7: **procedure** DiscretizeOperator( $\mathcal{L}, \mathcal{G}_h$ )
- 8:     Translate the differential operator  $\mathcal{L}$  into a discrete operator  $\mathcal{L}_h$  using mimetic principles
- 9:     Ensure that  $\mathcal{L}_h$  mimics the conservation and symmetry properties of  $\mathcal{L}$
- 10:     **return**  $\mathcal{L}_h$
- 11: **end procedure**
- 12: **procedure** ApplyBoundaryConditions( $\mathcal{L}_h, \mathcal{B}, \mathcal{G}_h$ )
- 13:     Modify  $\mathcal{L}_h$  on the boundary of  $\mathcal{G}_h$  to incorporate the boundary conditions  $\mathcal{B}$
- 14:     **return** Modified operator  $\mathcal{L}_h^*$
- 15: **end procedure**
- 16: **procedure** SolveDiscreteProblem( $\mathcal{L}_h^*, f, \mathcal{G}_h$ )
- 17:     Discretize  $f$  over  $\mathcal{G}_h$  to obtain  $f_h$
- 18:     Solve the discrete system  $\mathcal{L}_h^* u_h = f_h$  for  $u_h$
- 19:     **return**  $u_h$
- 20: **end procedure**
- 21:  $\mathcal{G}_h \leftarrow$  DiscretizeDomain( $\Omega, h$ )
- 22:  $\mathcal{L}_h \leftarrow$  DiscretizeOperator( $\mathcal{L}, \mathcal{G}_h$ )
- 23:  $\mathcal{L}_h^* \leftarrow$  ApplyBoundaryConditions( $\mathcal{L}_h, \mathcal{B}, \mathcal{G}_h$ )
- 24:  $u_h \leftarrow$  SolveDiscreteProblem( $\mathcal{L}_h^*, f, \mathcal{G}_h$ )
- 25: Visualize and analyze  $u_h$  to assess the approximation to the continuous solution  $u$

The mathematical model for steady-state groundwater flow in a homogeneous, isotropic aquifer can be described by the POISSON equation:

$$\nabla^2 \phi = q, \tag{1}$$

where  $\phi(x, y)$  represents the hydraulic head, and  $q(x, y)$  denotes the spatial distribution of sources (positive values) and sinks (negative values), corresponding to injection and extraction wells, respectively. The LAPLACIAN operator,  $\nabla^2$ , is discretized using a mimetic finite difference approach to accurately capture the flow behavior across a grid of points within the domain.

The computational domain is discretized into a uniform grid with spacing  $h$ . The LAPLACIAN operator in two dimensions is approximated using second-order central differences, leading to a stencil that couples each grid point with its four immediate neighbors. For a grid of  $n \times n$  points, the discretized LAPLACIAN,  $\mathbf{L}$ , is constructed as follows:

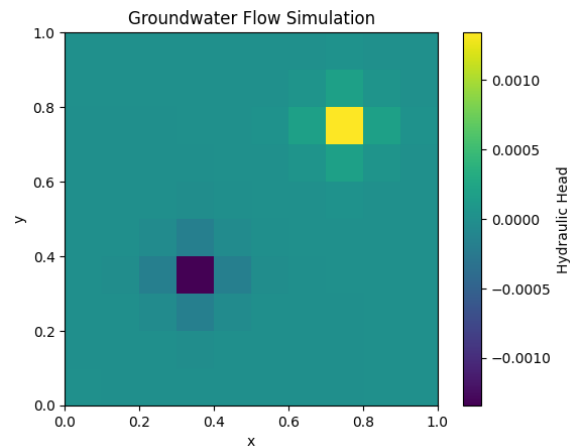
$$\mathbf{L} = \frac{1}{h^2} (\mathbf{L}_x \otimes \mathbf{I} + \mathbf{I} \otimes \mathbf{L}_y), \tag{2}$$

where  $\mathbf{L}_x$  and  $\mathbf{L}_y$  are the one-dimensional LAPLACIAN matrices along the  $x$  and  $y$  directions, respectively, and  $\mathbf{I}$  is the identity matrix. The KRONECKER product,  $\otimes$ , is used to construct the two-dimensional LAPLACIAN matrix from its one-dimensional counterparts.

DIRICHLET boundary conditions are applied to simulate specific hydraulic head values along the domain's boundaries. The boundary conditions are incorporated into the system by modifying the corresponding rows in the LAPLACIAN matrix, effectively overriding the equation at those points with the prescribed head values.

The resulting linear system,  $\mathbf{L}\phi = \mathbf{q}$ , where  $\mathbf{q}$  is the vector representing source/sink terms at grid points, is solved for the hydraulic head distribution,  $\phi$ , using sparse matrix techniques for efficiency.

The Python implementation utilizes the SciPy library for sparse linear algebra operations, a conceptual algorithm is illustrated in Algorithm 2. The simulation parameters, including grid resolution ( $n$ ) and spacing ( $h$ ), along with the distribution of sources and sinks ( $q$ ), define the problem setup. The groundwater flow equation is solved, and the resulting hydraulic head distribution is visualized, as depicted in Figure 3.



**FIGURE 3.** Simulated hydraulic head distribution in a domain with injection and extraction wells, demonstrating the capability of mimetic finite difference methods to model groundwater flow.

The mimetic finite difference approach offers a robust framework for simulating groundwater flow, providing key insights into the behavior of subsurface water movement influenced by anthropogenic activities. Future work will extend this methodology to more complex scenarios, including heterogeneous aquifer properties and transient flow conditions, further enhancing our capacity to manage and protect vital water resources.

Generalizing the approach to a 3D environment involves extending the concepts of constructing differential operators, applying boundary conditions, and solving the problem to accommodate the additional spatial dimension, as described in Algorithm 3. This entails dealing with a three-dimensional

**Algorithm 2** Solving Physical Problems Using Mimetic Finite Differences

- 1: **Input:** Problem parameters including domain size  $n$ , grid spacing  $h$ , source terms  $q$ , and boundary conditions  $\mathcal{B}$
- 2: **Output:** Solution to the physical problem, represented by variable  $u$
- 3: **function** ConstructOperator( $n, h$ , operator type)
- 4:     Construct a sparse matrix representation of a specified operator (e.g., Laplacian) in two dimensions
- 5:     Discretize the operator using a scheme appropriate for its type, scaled by  $\frac{1}{h^2}$  if necessary
- 6:     **return** Operator matrix
- 7: **end function**
- 8: **function** ApplyBoundaryConditions( $\mathcal{O}, \mathcal{B}, n$ )
- 9:     Modify operator matrix  $\mathcal{O}$  to incorporate specified boundary conditions  $\mathcal{B}$
- 10:     Adjust matrix entries according to the boundary conditions for the problem
- 11:     **return** Modified operator matrix  $\mathcal{O}$
- 12: **end function**
- 13: **function** SolvePDE( $\mathcal{O}, q, \mathcal{B}, n, h$ )
- 14:     Formulate the global operator matrix  $\mathcal{O}$  using ConstructOperator for the problem at hand
- 15:      $\mathcal{O} \leftarrow$  ApplyBoundaryConditions( $\mathcal{O}, \mathcal{B}, n$ )
- 16:     Prepare the right-hand side vector  $q$  representing source terms or forcing functions
- 17:     Solve the linear system  $\mathcal{O}u = q$  for the variable  $u$
- 18:     **return**  $u$  appropriately reshaped for the problem's geometry
- 19: **end function**
- 20: Determine the problem's parameters ( $n, h, q, \mathcal{B}$ ) based on the physical context
- 21: Choose the operator type based on the physical laws governing the problem (e.g., Laplacian for diffusion processes)
- 22:  $\mathcal{O} \leftarrow$  ConstructOperator( $n, h$ , operator type)
- 23:  $u \leftarrow$  SolvePDE( $\mathcal{O}, q, \mathcal{B}, n, h$ )
- 24: Optionally, visualize the solution  $u$  to interpret the physical phenomena under study

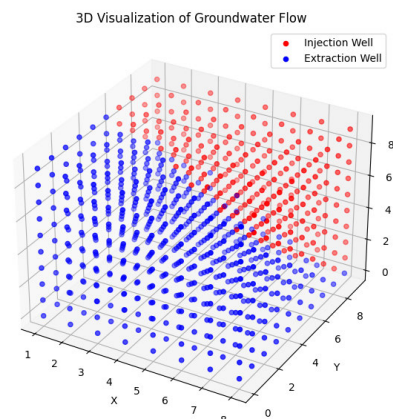
grid and considering how boundary conditions and source terms are specified in this expanded context.

This approach, as demonstrated in the simulated environment depicted in Figures 4 and 5, involves the construction of a 3D Laplacian matrix to model diffusion processes within a volumetric domain. The method extends the principles of mimetic discretization, previously applied to 2D scenarios, to accommodate the complexity of 3D spaces.

In the experiment we simulate a 3D groundwater flow by constructing a 3D LAPLACIAN matrix, applying boundary conditions, and solving the corresponding linear system. The analysis is simplified to displaying a slice of the 3D domain for illustrative purposes.

**Algorithm 3** Solving 3D Physical Problems Using Mimetic Finite Differences

- 1: **Input:** Problem parameters including 3D domain sizes  $n_x, n_y, n_z$ , grid spacings  $h_x, h_y, h_z$ , source terms  $q$ , and boundary conditions  $\mathcal{B}$
- 2: **Output:** Solution to the 3D physical problem, represented by variable  $u$
- 3: **function** Construct3DOperator( $n_x, n_y, n_z, h_x, h_y, h_z$ , operator type)
- 4:     Construct sparse matrix representations of the specified operator (e.g., Laplacian) in three dimensions
- 5:     Discretize the operator using schemes appropriate for its type, scaled by  $\frac{1}{h_x^2}, \frac{1}{h_y^2}, \frac{1}{h_z^2}$  as necessary
- 6:     Combine the discretized operators for each dimension to form a global operator matrix for the 3D problem
- 7:     **return** Global operator matrix for the 3D domain
- 8: **end function**
- 9: **function** Apply3DBoundaryConditions( $\mathcal{O}, \mathcal{B}, n_x, n_y, n_z$ )
- 10:     Modify the global operator matrix  $\mathcal{O}$  to incorporate specified 3D boundary conditions  $\mathcal{B}$
- 11:     Adjust matrix entries based on boundary conditions specific to 3D problems
- 12:     **return** Modified global operator matrix  $\mathcal{O}$
- 13: **end function**
- 14: **function** Solve3DPDE( $\mathcal{O}, q, \mathcal{B}, n_x, n_y, n_z, h_x, h_y, h_z$ )
- 15:     Formulate the global operator matrix  $\mathcal{O}$  for the 3D problem
- 16:      $\mathcal{O} \leftarrow$  Apply3DBoundaryConditions( $\mathcal{O}, \mathcal{B}, n_x, n_y, n_z$ )
- 17:     Prepare the right-hand side vector  $q$  representing 3D source terms or forcing functions
- 18:     Solve the 3D linear system  $\mathcal{O}u = q$  for the variable  $u$
- 19:     **return**  $u$  reshaped to the 3D domain geometry
- 20: **end function**
- 21: Determine the 3D problem's parameters based on the physical context
- 22: Choose the operator type suitable for the governing physical laws of the problem
- 23:  $\mathcal{O} \leftarrow$  Construct3DOperator( $n_x, n_y, n_z, h_x, h_y, h_z$ , operator type)
- 24:  $u \leftarrow$  Solve3DPDE( $\mathcal{O}, q, \mathcal{B}, n_x, n_y, n_z, h_x, h_y, h_z$ )
- 25: Optionally, visualize the solution  $u$  in 3D to interpret the physical phenomena being modeled



**FIGURE 4.** 3D visualization of groundwater flow.

The spatial and temporal resolution parameters, such as grid spacing and time steps, are set to balance computational feasibility with the need for accuracy, as informed by convergence studies reported in similar research. Furthermore,

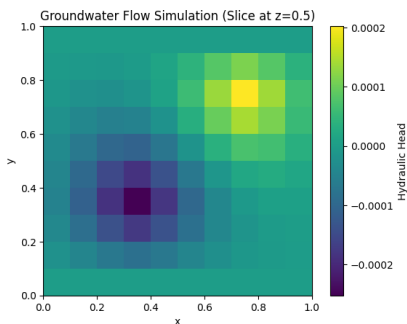


FIGURE 5. Groundwater flow simulation (slice at  $z = 0.5$ ).

the choice of boundary conditions and problem setups, such as flow around a circular cylinder, are designed to test the robustness of our mimetic discretization methods under conditions known to present complex flow patterns, thereby validating our approach against challenging practical applications.

### V. APPLICATIONS IN AEROSPACE ENGINEERING

The mimetic discretization framework, with its ability to accurately capture the complex behavior of fluid flows while preserving the essential physical properties of the system, holds significant promise for applications in aerospace engineering. One of the primary areas where mimetic methods can be applied is in the simulation of fluid flows around aircraft. The accurate modeling of aerodynamic flows is crucial for the design and optimization of aircraft components, such as wings, fuselages, and control surfaces.

Mimetic discretizations can be employed to solve the NAVIER-STOKES equations governing the fluid flow around an aircraft, taking into account the complex geometries and boundary conditions involved. By preserving the conservation laws and symmetries inherent in the continuous equations, mimetic methods can provide high-fidelity simulations of the flow field, including the prediction of lift, drag, and moment coefficients. These simulations can aid in the assessment of aircraft performance, stability, and control characteristics, enabling engineers to make informed design decisions.

In order to provide a clear and systematic representation of our computational approach, we present a detailed algorithm in 4 that presents the solution process for the NAVIER-STOKES equations using the mimetic discretization method. This algorithm illustrates the sequential steps involved in the simulation, emphasizing the order in which the equations are solved, the application of boundary conditions, and the integration over time.

Another potential application of mimetic discretizations in aerospace engineering is in the design optimization of aerodynamic components. The development of efficient and reliable optimization algorithms relies on the accurate evaluation of objective functions and constraints, which often involve the solution of fluid flow equations. Mimetic methods can be incorporated into optimization frameworks to provide

### Algorithm 4 Solution Algorithm for NAVIER-STOKES Equations Using Mimetic Discretization

- 1: **Input:** Initial conditions, physical and computational parameters
- 2: **Output:** Velocity fields, pressure distribution
- 3: **procedure** Initialize
- 4:     Define grid and discretization parameters
- 5:     Allocate memory for velocity, pressure, and auxiliary variables
- 6: **end procedure**
- 7: **procedure** DiscretizeDomain
- 8:     Apply mimetic operators to discretize the NAVIER-STOKES equations
- 9: **end procedure**
- 10: **procedure** TimeStep
- 11:     **for** each time step **do**
- 12:         Apply boundary conditions
- 13:         Solve momentum equations
- 14:         Solve continuity equation for pressure correction
- 15:         Check convergence
- 16:         **if** converged **then**
- 17:             **break**
- 18:         **end if**
- 19:     **end for**
- 20: **end procedure**
- 21: Initialize
- 22: DiscretizeDomain
- 23: TimeStep

accurate and physically consistent flow solutions, enabling the exploration of large design spaces and the identification of optimal configurations.

For example, mimetic discretizations can be used in shape optimization problems, where the goal is to determine the optimal shape of an aircraft component, such as a wing or a nacelle, to minimize drag or maximize lift. By coupling mimetic methods with gradient-based or evolutionary optimization algorithms, engineers can efficiently navigate the design space and arrive at optimized geometries that satisfy the desired performance criteria.

Furthermore, mimetic discretizations can be applied to the study of fluid-structure interactions (FSI) in aerospace systems. FSI problems involve the coupled analysis of fluid flows and structural deformations, which is essential for understanding the behavior of flexible aircraft components, such as wings or turbine blades. Mimetic methods can be used to discretize the fluid domain, while compatible structural discretizations can be employed for the solid domain. The coupling between the fluid and structural solvers can be facilitated by the consistent treatment of interface conditions and the preservation of conservation properties afforded by mimetic discretizations.

The application of mimetic methods to FSI problems in aerospace engineering can lead to more accurate predictions



of the aeroelastic behavior of aircraft, including the onset of flutter, the response to gust loads, and the impact of structural flexibility on aerodynamic performance. These insights can inform the design of lighter, more efficient, and safer aircraft structures.

In addition to these specific applications, mimetic discretizations can be used in a wide range of aerospace engineering problems involving fluid flows, such as the analysis of propulsion systems, the simulation of hypersonic flows, and the study of atmospheric entry vehicles. The ability of mimetic methods to handle complex geometries, accurately capture shock waves and other discontinuities, and preserve important physical properties makes them well-suited for these challenging applications.

To fully harness the potential of mimetic discretizations in aerospace engineering, further research is needed to develop efficient and scalable implementations of these methods, particularly for large-scale problems involving millions of degrees of freedom. The integration of mimetic methods with high-performance computing platforms, such as parallel processors and graphics processing units (GPUs), can enable the simulation of more complex and realistic aerospace systems.

Moreover, the combination of mimetic discretizations with other advanced numerical techniques, such as adaptive mesh refinement, higher-order schemes, and immersed boundary methods, can further enhance the accuracy and efficiency of aerospace simulations. The development of multidisciplinary design optimization frameworks that incorporate mimetic methods for fluid flow analysis, along with other disciplinary models, such as structural mechanics and heat transfer, can lead to a more holistic and integrated approach to aircraft design.

For instance, in groundwater flow simulations, mimetic discretizations inherently ensure the preservation of physical conservation laws—such as mass conservation—which are often only approximately maintained in standard finite difference approaches. This is particularly critical in scenarios involving complex boundary conditions and heterogeneous aquifer properties, where traditional methods might fail to accurately capture the complex dynamics of the flow. Moreover, unlike conventional discretization techniques, which may introduce significant numerical diffusion or fail to preserve geometric properties, mimetic schemes inherently maintain the orthogonality and curl-free nature of flow fields, critical for accurately predicting aerodynamic forces and moments. This capability is not just theoretically advantageous but has practical implications in reducing computational overhead and enhancing simulation accuracy, which are vital for the iterative design processes in aerospace engineering.

That is, the mimetic discretization framework holds significant promise for advancing the state-of-the-art in aerospace engineering simulations. By providing accurate, physically consistent, and stable numerical schemes for fluid flow problems, mimetic methods can contribute to the design

of more efficient, reliable, and high-performance aircraft. The continued research and development of mimetic discretizations, along with their integration into multidisciplinary design optimization frameworks, can revolutionize the way aerospace systems are designed and analyzed, leading to significant advancements in the field.

### A. HEXASCALE COMPUTING AND ITS IMPLICATIONS

The advent of hexascale computing, characterized by systems capable of performing at least one hexaflop ( $10^{18}$  floating-point operations per second), presents both opportunities and challenges for the application of mimetic discretization methods in aerospace engineering. The immense computational power offered by hexascale systems can enable the simulation of more complex and realistic aerospace problems, providing unprecedented insights into the behavior of fluid flows and their interactions with aircraft structures.

One of the key benefits of hexascale computing for mimetic discretizations is the ability to handle extremely large and detailed computational grids. With the increased memory and processing power available, engineers can discretize the fluid domain using much finer resolutions, capturing intricate flow features and small-scale phenomena that may have been previously unresolved. This enhanced resolution can lead to more accurate predictions of aerodynamic forces, heat transfer, and other critical quantities of interest in aerospace simulations.

Moreover, hexascale computing can facilitate the use of higher-order mimetic schemes, which can provide improved accuracy and convergence properties compared to lower-order methods. The increased computational resources can accommodate the additional degrees of freedom and the more complex stencil computations associated with higher-order discretizations. This can result in more precise simulations of fluid flows, particularly in regions with strong gradients or discontinuities, such as shock waves or boundary layers.

However, the transition to hexascale computing also poses significant challenges for the efficient implementation and scalability of mimetic discretization methods. The massive parallelism and hierarchical memory structures of hexascale systems require careful design and optimization of the numerical algorithms and data structures used in mimetic methods. The development of efficient domain decomposition strategies, load balancing techniques, and communication protocols becomes crucial to fully harness the power of hexascale computing.

One approach to address these challenges is the use of hybrid parallel programming models, such as the combination of message passing interface (MPI) for inter-node communication and OpenMP or CUDA for intra-node parallelism. By exploiting the different levels of parallelism available in hexascale systems, mimetic methods can be optimized for both strong and weak scaling, enabling the efficient utilization of the vast computing resources.

Another important consideration in the context of hexascale computing is the development of fault-tolerant

algorithms and resilient solution strategies. With the increasing complexity and scale of hexascale systems, the probability of hardware failures or silent data corruptions becomes higher. Mimetic discretizations should be designed to incorporate error detection and correction mechanisms, such as checkpointing, redundancy, or algorithm-based fault tolerance (ABFT), to ensure the reliability and integrity of the simulations in the presence of faults.

The availability of hexascale computing also opens up new possibilities for the integration of mimetic discretizations with data-driven approaches and machine learning techniques. The vast amounts of data generated by high-fidelity simulations can be leveraged to train predictive models, surrogate models, or reduced-order models that can accelerate the design optimization process. Machine learning algorithms can be used to identify patterns, correlations, and anomalies in the simulation data, providing valuable insights for the design and analysis of aerospace systems.

Furthermore, hexascale computing can enable the coupling of mimetic discretizations with other high-fidelity simulation techniques, such as large eddy simulations (LES) or direct numerical simulations (DNS), to capture the multiscale and multiphysics nature of aerospace flows. The increased computational power can allow for the resolution of a wider range of spatial and temporal scales, enabling the study of complex turbulent flows, flow-induced vibrations, and other coupled phenomena.

To fully realize the potential of mimetic discretizations in the era of hexascale computing, ongoing research and development efforts are necessary. This includes the development of scalable solver algorithms, such as multigrid methods or domain decomposition techniques, that can efficiently solve the large linear systems arising from mimetic discretizations. The adaptation of mimetic methods to emerging hardware architectures, such as many-core processors or reconfigurable computing platforms, can further enhance their performance and energy efficiency.

Moreover, the establishment of standard benchmarks, validation cases, and performance metrics for mimetic discretizations in the context of hexascale computing can facilitate the assessment and comparison of different numerical schemes and implementations. Collaboration between the aerospace engineering community, applied mathematicians, and computer scientists is essential to address the interdisciplinary challenges associated with the deployment of mimetic methods on hexascale systems.

To sum up, the advent of hexascale computing presents significant opportunities for advancing the application of mimetic discretization methods in aerospace engineering. The increased computational power and memory capacity of hexascale systems can enable the simulation of more complex and realistic fluid flow problems, leading to improved accuracy and physical fidelity. However, the efficient implementation and scalability of mimetic methods on hexascale architectures require careful consideration of parallel programming models, fault tolerance, and algorithm

design. The integration of mimetic discretizations with data-driven approaches and other high-fidelity simulation techniques can further enhance their predictive capabilities and support the design optimization of aerospace systems.

## VI. DISCUSSION

The results presented in this study highlight the significance of mimetic discretization methods in the field of computational fluid dynamics, particularly in the context of the NAVIER-STOKES equations. The theoretical foundations presented in this work, encompassing the isomorphism theorems, subalgebras, ideals, and short exact sequences, provide a comprehensive framework for understanding the algebraic and topological properties of discrete function spaces arising from mimetic discretizations.

The isomorphism theorems, as applied to the mimetic gradient and divergence operators, reveal the intricate relationships between the kernel and image spaces of these operators. These findings have far-reaching implications for the analysis and design of numerical schemes based on mimetic discretizations. By characterizing the structure of the discrete function spaces and their connection to the continuous realm, the isomorphism theorems provide a powerful tool for assessing the accuracy, stability, and convergence properties of mimetic schemes.

Moreover, the exploration of subalgebras, ideals, and their quotients within the context of mimetic discretizations opens up new avenues for the development of algebraic techniques in the analysis of discrete systems. These abstract structures offer a rich framework for characterizing the behavior of discrete function spaces and their relationship to the underlying physical phenomena. The insights gained from this algebraic perspective can guide the design of novel mimetic schemes that better capture the essential features of the continuous equations.

The examination of short exact sequences involving mimetic operators further reinforces the parallels between the discrete and continuous settings. By establishing the exactness of these sequences and the validity of the isomorphism theorems, this study lays the groundwork for a deeper understanding of the mathematical properties of mimetic discretizations. These findings have direct implications for the analysis of the convergence, stability, and error behavior of mimetic schemes, enabling the development of more robust and accurate numerical methods.

The practical application of mimetic finite difference methods to the simulation of groundwater flow demonstrates the potential of mimetic discretizations in tackling real-world problems. The presented numerical scheme showcases the ability of mimetic methods to accurately capture the complex behavior of subsurface water movement influenced by injection and extraction wells. This example highlights the effectiveness of mimetic discretizations in preserving the essential physical properties of the system, such as conservation laws and symmetries, leading to more reliable and physically consistent simulations.

Specifically, the enhanced precision and adherence to physical laws in our computational models allow for more accurate simulations of fluid dynamics in engineering systems, such as aerodynamics in automotive and aerospace industries and fluid flow in energy systems like oil and gas pipelines. For example, the improved modeling of airflows around vehicle bodies can lead to designs that minimize drag and improve fuel efficiency. Similarly, in civil engineering, our approach can be applied to simulate water flow through dams or urban drainage systems, enhancing designs to prevent floods. These applications demonstrate the method's practical relevance and potential to contribute significantly to advancements in technology and infrastructure.

For instance, when applied to the NAVIER-STOKES equations, mimetic discretization not only accurately captures complex flow patterns but also ensures the conservation of mass and momentum better than traditional FEM or FVM, particularly in simulations involving sharp gradients and discontinuities. Additionally, unlike spectral methods, which can suffer from GIBBS phenomenon near discontinuities, our approach maintains stability without sacrificing spatial resolution. These comparisons underscore the distinct advantages of mimetic discretizations in handling complex physical phenomena, making them highly applicable to a broad range of engineering problems.

However, it is important to acknowledge the limitations and challenges associated with mimetic discretization methods. The construction of mimetic operators requires careful consideration of the discrete function spaces and their compatibility with the underlying physical principles. The choice of appropriate function spaces and the design of suitable discrete operators can be non-trivial tasks, especially for complex geometries and boundary conditions. Furthermore, the efficient implementation of mimetic schemes may require specialized numerical linear algebra techniques and data structures to handle the resulting sparse matrices.

Despite these challenges, the potential benefits of mimetic discretizations in computational fluid dynamics are significant. By providing a rigorous mathematical foundation for the development of structure-preserving numerical schemes, mimetic methods offer the promise of improved accuracy, stability, and efficiency in the simulation of fluid flows. The insights gained from this study can guide the development of novel mimetic schemes tailored to specific applications, such as turbulence modeling, multiphase flows, and fluid-structure interactions.

Beyond traditional engineering fields, these methods can be very important in areas like environmental science, where they can enhance the modeling of complex natural systems such as climate dynamics and oceanography. For example, mimetic discretizations are instrumental in simulating ocean currents and climate patterns with higher accuracy, helping in predicting climate changes more reliably. In medical engineering, these techniques contribute to the simulation of blood flow through arteries, assisting in the design of medical devices and in understanding cardiovascular diseases. The

ability of mimetic discretization to preserve essential physical properties in simulations makes it highly valuable for pharmaceutical industries as well, where it is used in the modeling of mixing processes to ensure uniformity and efficacy in the production of medicinal solutions.

Future research directions in this field are manifold. The extension of mimetic discretizations to more complex physical systems and the incorporation of advanced numerical techniques, such as adaptive mesh refinement and parallel computing, present exciting opportunities for further advancements. The exploration of the discrete DE RHAM cohomology and the discrete HODGE theory can provide a deeper understanding of the topological properties of discrete function spaces and their role in the analysis of numerical methods for partial differential equations.

Moreover, the integration of mimetic discretizations with other computational approaches, such as finite element methods and spectral methods, can lead to the development of hybrid schemes that leverage the strengths of each approach. The combination of mimetic methods with data-driven techniques, such as machine learning and uncertainty quantification, can open up new possibilities for the data-informed simulation and optimization of fluid systems.

## VII. CONCLUSION AND FUTURE WORK

The journey through the intricate landscapes of computational fluid dynamics (CFD) and mimetic discretization methodologies has unfolded a rich tapestry of mathematical theories and computational strategies aimed at the accurate representation of physical phenomena governed by the NAVIER-STOKES equations. The essence of this exploration lies in the relentless pursuit of numerical techniques that not only promise precision but also fidelity to the underlying physical laws and geometric, topological, and algebraic properties intrinsic to fluid dynamics.

Mimetic discretization has illuminated paths that bridge the discrete and continuous realms of mathematical modeling. Through the adept definition and implementation of discrete analogs for gradient and divergence operators, mimetic discretization ensures that these surrogates of differentiation adhere as closely as possible to their continuous counterparts. This adherence is paramount, not just for the accuracy of simulations but for the preservation of physical laws within the computational domain.

The exploration of the algebraic and topological underpinnings of discrete function spaces has unraveled the profound connections between the kernel and image spaces of mimetic operators. The insights gleaned from these investigations are foundational, offering a fresh lens through which the symbiosis of discrete and continuous mathematical models is viewed. This study further delves into the realms of sub-algebras, ideals, their quotients, and short exact sequences, thus enriching the algebraic framework within which mimetic discretizations are conceptualized and understood.

Beyond the theoretical allure, the ramifications of this study extend into the practical sphere, influencing the

development and refinement of numerical schemes for tackling the NAVIER-STOKES equations. The elucidation of the structural attributes of mimetic discretizations lays down a strong groundwork for advancing numerical methods that are not merely accurate but inherently tuned to the preservation of the physical and mathematical essence of the phenomena they seek to model.

The analytical insights into mimetic discretizations have the potential to impact a diverse spectrum of applications. From the forecasting of weather phenomena and ocean modeling to the design and optimization of aerospace vehicles and the study of complex biological flows, the utility of these insights is manifold.

The applications of the advanced mimetic discretization techniques developed in this study extend to several critical real-world problems, underscoring their practical relevance beyond theoretical constructs. For instance, the enhanced modeling of the NAVIER-STOKES equations can significantly improve the simulation of fluid flow in industrial processes such as chemical mixing and petroleum extraction, where understanding the behavior of non-homogeneous and anisotropic flows is crucial. Additionally, our model has potential applications in environmental engineering, particularly in the simulation of water flow in rivers and estuaries, which is essential for flood prediction and the management of water resources. The ability of our methods to accurately capture complex fluid dynamics also makes them valuable for designing more efficient and safer air and watercraft by enabling precise predictions of aerodynamic and hydrodynamic performance under various operating conditions. By bridging the gap between theoretical advancements and practical engineering challenges, this work illustrates a direct pathway for the implementation of sophisticated Computational Fluid Dynamics (CFD) techniques in solving tangible and impactful engineering problems.

The study presented in this paper focuses on the application of mimetic discretization techniques to solve the NAVIER-STOKES equations, which are fundamental in modeling fluid dynamics. This application is crucial for several engineering fields where fluid behavior under different conditions must be accurately predicted. For example, in aerospace engineering, our methods can be used to simulate airflow over aircraft wings to optimize design for improved efficiency and safety. In the automotive industry, similar simulations help in refining the aerodynamics of vehicles for better fuel efficiency and stability. Additionally, our approach can be employed in the environmental sector to model complex fluid interactions in natural water bodies, aiding in pollution control and disaster management strategies such as flood mitigation. By providing a robust computational tool to simulate real-world fluid dynamics, our research supports innovative solutions to engineering challenges, ensuring that theoretical advancements are translated into practical benefits.

In conclusion, our study not only advances the theoretical framework of mimetic discretizations but also underscores

their practical utility in addressing complex fluid dynamics scenarios, particularly in engineering applications involving the NAVIER-STOKES equations. The physical insights gained from our simulations reveal the effectiveness of our refined mimetic methods in capturing critical phenomena such as turbulence, boundary layer effects, and anisotropic flow behavior, which are crucial for the design and optimization of hydraulic systems, aerospace components, and environmental monitoring equipment.

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## REFERENCES

- [1] J. Brzenski and J. E. Castillo, “Solving Navier–Stokes with mimetic operators,” *Comput. Fluids*, vol. 254, Mar. 2023, Art. no. 105817.
- [2] J. Corbino and J. E. Castillo, “High-order mimetic finite-difference operators satisfying the extended Gauss divergence theorem,” *J. Comput. Appl. Math.*, vol. 364, Jan. 2020, Art. no. 112326, doi: [10.1016/j.cam.2019.06.042](https://doi.org/10.1016/j.cam.2019.06.042).
- [3] J. E. Castillo and R. D. Grone, “A matrix analysis approach to higher-order approximations for divergence and gradients satisfying a global conservation law,” *SIAM J. Matrix Anal. Appl.*, vol. 25, no. 1, pp. 128–142, Jan. 2003, doi: [10.1137/s0895479801398025](https://doi.org/10.1137/s0895479801398025).
- [4] J. E. Castillo and G. F. Miranda, *Mimetic Discretization Methods*. Boca Raton, FL, USA: CRC Press, 2013.
- [5] J. de la Puente, M. Ferrer, M. Hanzich, J. E. Castillo, and J. M. Cela, “Mimetic seismic wave modeling including topography on deformed staggered grids,” *Geophysics*, vol. 79, no. 3, pp. T125–T141, May 2014.
- [6] M. Abouali and J. E. Castillo, “Solving Poisson equation with Robin boundary condition on a curvilinear mesh using high order mimetic discretization methods,” *Math. Comput. Simul.*, vol. 139, pp. 23–36, Sep. 2017, doi: [10.1016/j.matcom.2014.10.004](https://doi.org/10.1016/j.matcom.2014.10.004).
- [7] J. Villamizar, L. Mendoza, G. Calderón, O. Rojas, and J. E. Castillo, “High order mimetic differences applied to the convection–diffusion equation: A matrix stability analysis,” *GEM Int. J. Geomathematics*, vol. 14, no. 1, p. 26, Dec. 2023.
- [8] M. Shashkov, *Conservative Finite-Difference Methods on General Grids*. Boca Raton, FL, USA: CRC Press, 1995.
- [9] J. Hyman, J. Morel, M. Shashkov, and S. Steinberg, “Mimetic finite difference methods for diffusion equations,” *Comput. Geosci.*, vol. 6, pp. 333–352, Sep. 2001.
- [10] O. Rojas, S. Day, J. Castillo, and L. A. Dalguer, “Modelling of rupture propagation using high-order mimetic finite differences,” *Geophys. J. Int.*, vol. 172, no. 2, pp. 631–650, Feb. 2008.
- [11] C. Bazan, M. Abouali, J. Castillo, and P. Blomgren, “Mimetic finite difference methods in image processing,” *Comput. Appl. Math.*, vol. 30, no. 3, pp. 701–720, 2011.
- [12] J. Blanco, O. Rojas, C. Chacón, J. M. Guevara-Jordan, and J. Castillo, “Tensor formulation of 3-D mimetic finite differences and applications to elliptic problems,” *Electron. Trans. Numer. Anal.*, vol. 45, pp. 457–475, Dec. 2016.
- [13] H.-O. Kreiss and G. Scherer, “Finite element and finite difference methods for hyperbolic partial differential equations,” in *Mathematical Aspects of Finite Elements in Partial Differential Equations*. New York, NY, USA: Academic, 1974, pp. 195–212.
- [14] K. Lipnikov, G. Manzini, and M. Shashkov, “Mimetic finite difference method,” *J. Comput. Phys.*, vol. 257, pp. 1163–1227, Jan. 2014.
- [15] P. B. Bochev and J. M. Hyman, “Principles of mimetic discretizations of differential operators,” in *Compatible Spatial Discretizations*, D. N. Arnold, P. B. Bochev, R. B. Lehoucq, R. A. Nicolaides, and M. Shashkov, Eds., New York, NY, USA: Springer, 2006, pp. 89–119, doi: [10.1007/0-387-38034-5\\_5](https://doi.org/10.1007/0-387-38034-5_5).



- [16] J. Corbino, M. A. Dumett, and J. E. Castillo, "MOLE: Mimetic operators library enhanced," *J. Open Source Softw.*, vol. 9, no. 99, p. 6288, Jul. 2024, doi: [10.21105/joss.06288](https://doi.org/10.21105/joss.06288).
- [17] D. Patel, D. Ray, M. R. A. Abdelmalik, T. J. R. Hughes, and A. A. Oberai, "Variationally mimetic operator networks," *Comput. Methods Appl. Mech. Eng.*, vol. 419, Feb. 2024, Art. no. 116536.
- [18] Z. Shi, N. S. Gulgec, A. S. Berahas, S. N. Pakzad, and M. Takác, "Finite difference neural networks: Fast prediction of partial differential equations," in *Proc. 19th IEEE Int. Conf. Mach. Learn. Appl. (ICMLA)*, Dec. 2020, pp. 130–135.
- [19] C.-C. Ye, P.-J.-Y. Zhang, Z.-H. Wan, R. Yan, and D.-J. Sun, "Accelerating CFD simulation with high order finite difference method on curvilinear coordinates for modern GPU clusters," *Adv. Aerodynamics*, vol. 4, no. 1, p. 7, Dec. 2022.
- [20] M. S. Arif, K. Abodayeh, and Y. Nawaz, "Explicit computational analysis of unsteady Maxwell nanofluid flow on moving plates with stochastic variations," *Int. J. Thermofluids*, vol. 23, Aug. 2024, Art. no. 100755, doi: [10.1016/j.ijft.2024.100755](https://doi.org/10.1016/j.ijft.2024.100755). [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S2666202724001976>
- [21] M. S. Arif, K. Abodayeh, and Y. Nawaz, "Dynamic simulation of non-newtonian boundary layer flow: An enhanced exponential time integrator approach with spatially and temporally variable heat sources," *Open Phys.*, vol. 22, no. 1, 2024, Art. no. 20240034.
- [22] M. S. Arif, K. Abodayeh, and Y. Nawaz, "Numerical modeling of mixed convective nanofluid flow with fractal stochastic heat and mass transfer using finite differences," *Frontiers Energy Res.*, vol. 12, 2024, Art. no. 1373079.
- [23] A. Palha and M. Gerritsma, "Mimetic spectral element method for Hamiltonian systems," 2015, *arXiv:1505.03422*.
- [24] J. de Curtò and I. de Zarzà, "Spectral properties of mimetic operators for robust Fluid–Structure interaction in the design of aircraft wings," *Mathematics*, vol. 12, no. 8, p. 1217, Apr. 2024, doi: [10.3390/math12081217](https://doi.org/10.3390/math12081217).
- [25] M. Vázquez, G. Houzeaux, S. Koric, A. Artigues, J. Aguado-Sierra, R. Arís, D. Mira, H. Calmet, F. Cucchietti, H. Owen, A. Taha, E. D. Burness, J. M. Cela, and M. Valero, "Alya: Multiphysics engineering simulation toward exascale," *J. Comput. Sci.*, vol. 14, pp. 15–27, May 2016, doi: [10.1016/j.jocs.2015.12.007](https://doi.org/10.1016/j.jocs.2015.12.007).



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