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COMPARATIVE ANALYSIS OF THE NUMERICAL SOLUTION OF THE DIFFUSION EQUATION IN PLANTS USING AUTOMATIC DIFFERENTIATION AND GRID METHODS

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ABSTRACT

This paper presents a numerical investigation of the diffusion equation that models heat transfer in plant tissues, with a particular focus on a comparative analysis of two computational approaches: automatic differentiation and the classical grid-based finite difference method. Diffusive transport is a fundamental mechanism in plant physiology, especially under extreme environmental conditions where the efficiency of heat and mass exchange plays a critical role in plant survival and adaptation. The primary objective of this study is to evaluate and compare the accuracy, computational efficiency, and stability of the two methods in solving a one-dimensional heat transfer model. The problem is formulated alongside a numerical experiment in which solutions obtained via automatic differentiation—implemented within machine learning frameworks—are benchmarked against results produced by the traditional finite difference approach. The findings underscore the strengths and limitations of each method within the context of biophysical modeling. Furthermore, the results suggest a promising potential for integrating both approaches into hybrid computational schemes to enhance the analysis of thermal and diffusive phenomena in biological systems.

KEYWORDS

diffusion, heat transfer, automatic differentiation, grid-based method, numerical modeling.

1. INTRODUCTION

Diffusion processes and heat transfer are fundamental to plant physiology, enabling adaptation to changing environmental conditions—particularly in extreme climatic zones. These processes are especially critical for succulent plants, which, due to their unique morphological and physiological features, are capable of efficiently conserving moisture and regulating internal temperature. Accurate mathematical modeling of heat and mass transfer in biological tissues necessitates the use of numerical methods that ensure both precision and solution stability (Hajrulla et al., 2023). Classical numerical techniques, such as finite difference grid-based methods, are widely employed for solving heat transfer and diffusion equations due to their established reliability and ease of implementation (Morton & Mayers, 2005). In recent years, there has been a growing interest in automatic differentiation techniques, which offer powerful tools for efficient gradient computation and the acceleration of numerical algorithms—particularly in modern computational platforms and machine learning frameworks (Baydin et al., 2018). Despite these advancements, comparative studies evaluating these methods within the specific context of biophysical modeling of heat and diffusion in plant tissues remain scarce. The integration of classical and modern approaches holds significant promise for the development of hybrid models that more accurately capture the complex structure of biological systems and the dynamics of nonlinear processes (Raissi, Perdikaris, & Karniadakis, 2019). In this context, the primary objective of the present study is to develop and conduct a comparative analysis of numerical methods for solving the one-dimensional heat diffusion equation, taking into account the physico-chemical properties of plant tissues. The focus is placed on two approaches: automatic differentiation techniques and the classical grid-based method. To achieve this objective, the following tasks are undertaken:

1) Formulate a mathematical model of heat transfer and diffusion that adequately reflects the biophysical conditions of plant tissues.
2) Implement numerical solutions of the model using both automatic differentiation and the classical grid-based method.
3) Perform a comparative analysis of the two approaches in terms of accuracy, stability, and computational efficiency.
4) Evaluate the potential of each method for application in biophysical modeling and the development of hybrid numerical schemes.

The outcomes of this study aim to contribute to both the theoretical and practical foundations of numerical modeling in plant biophysics. Ultimately, this may enhance our understanding of the mechanisms that enable plant adaptation to extreme climatic conditions.

2. METHODOLOGY

To numerically solve the one-dimensional heat diffusion equation in plant tissues, this study employs two primary approaches: the classical finite difference grid-based method and the automatic differentiation method.

The model under consideration is a one-dimensional heat transfer equation incorporating a diffusion term:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + Q(x,t)$$

where $u(x,t)$ denotes the temperature at position x and time t, D is the diffusion coefficient, and $Q(x,t)$ represents a heat source term accounting for the biophysical processes occurring within plant tissues. Boundary and initial conditions are prescribed taking into consideration the physico-chemical properties of the tissue and available experimental data .

2.1. GRID-BASED METOD

The finite difference method (grid-based metod) is employed to discretize the equation in both space and time. The spatial domain is divided into uniform steps of size Δx, while the temporal domain is discretized into steps of size Δt. Time integration is performed using an implicit scheme to ensure the stability of the solution. The implementation follows the classical approach as described in the literature (Patankar, 1980). Let L be a given differential operator acting on a function $u = u(x)$. We replace Lu with a discrete approximation $L_h u_h$, where $L_h u_h$ represents a linear combination of the values of the grid function u_h at a set of selected grid nodes. This set of nodes is referred to as a stencil**.**

$$L_h u_h(x) = \sum_{\varepsilon \in S(x)} A_h(x,\varepsilon)\, u_h(\varepsilon)$$

or

$$(L_h u_h)_i = \sum_{x_i \in S(x)} A_h(x_i, x_j)\, u_h(x_j)$$

Here, $A_h(x,\varepsilon)$ are the coefficients, h is the step size, and $S(x)$ denotes the stencil at the point x. Thus, this approach of replacing Lu with $L_h u_h$ is referred to as the approximation of a differential operator by a difference operator**.** The analysis of such an approximation is typically carried out at a fixed point x, that is, in the interior of the domain. If $u(x)$ is a continuous function, then the grid approximation satisfies the condition:

$$u_h(x) = u(x)$$

Before approximating the differential operator L with a difference operator, it is necessary to choose an appropriate stencil. That is, one must specify the set of neighboring grid points surrounding a given point x, at which the values of the function $u(x)$ can be used to approximate the action of the operator L.

2.2. AUTOMATIC DIFFERENTIATION

To solve the problem using automatic differentiation, a modern machine learning framework is employed, which supports accurate computation of derivatives via the chain rule (Baydin et al., 2018). The model and numerical solution are implemented within a differentiable environment, enabling parameter optimization and improving computational efficiency. The chain rule is a fundamental principle in calculus used to compute the derivative of a composite function. If a function y depends on u, which in turn depends on x, i.e., $y = f(u(x))$, then the derivative of y with respect to x is given by:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{\mathrm{d}f}{\mathrm{d}u} * \frac{\mathrm{d}u}{\mathrm{d}x}$$

In the context of automatic differentiation (AD), the chain rule serves as the core mechanism for propagating derivatives through computational graphs. Each operation in the graph is differentiable, and by applying the chain rule iteratively, AD frameworks compute exact derivatives of complex functions efficiently and accurately. Unlike symbolic differentiation, which can be computationally expensive, and numerical differentiation, which suffers from approximation errors, AD leverages the chain rule to combine the benefits of both — maintaining accuracy while enabling scalability. This makes it particularly useful in machine learning and scientific computing applications where gradients are essential.

3. EXPERIMENTAL RESULTS

Numerical experiments were conducted to solve the one-dimensional heat diffusion equation in plant tissues, and the results reveal notable differences in the behavior and performance of the automatic differentiation method and the classical grid-based method. Table 1 presents a comparative summary of the two methods in terms of mean absolute error, computation time, and numerical stability. Automatic differentiation demonstrated higher accuracy, with a lower mean absolute error (0.007 compared to 0.015 for the grid-based method), as well as greater robustness to changes in model parameters. However, its computational time was nearly twice as long (23.8 seconds vs. 12.4 seconds), primarily due to the additional overhead required for derivative computations.

Table 1. Comparative characteristics of the numerical methods

Method	Mean Absolute Error	Computation Time (s)	Maximum Deviation	Solution Stability
Grid-Based Method	0.015	12.4	0.045	Sensitive to parameters
Automatic Differentiation	0.007	23.8	0.018	High (robust performance)

Figure 1 illustrates the spatial distribution of temperature $u(x)$ at time $t = 0.5$, computed using both numerical methods. The curve obtained via automatic differentiation (red dashed line) exhibits greater smoothness and lacks the numerical oscillations observed in the solution produced by the grid-based method (blue solid line), particularly near the boundary points.

Analysis of the temporal evolution of the solution demonstrated that automatic differentiation allows the use of larger time steps without significant loss of accuracy, potentially reducing the overall computation time. At the same time, the classical grid-based method exhibits higher computational efficiency when small time steps are employed.The obtained results indicate that automatic differentiation is a promising approach for high-precision modeling of biophysical processes in plant tissues, whereas the grid-based method remains an effective tool under limited computational resources.

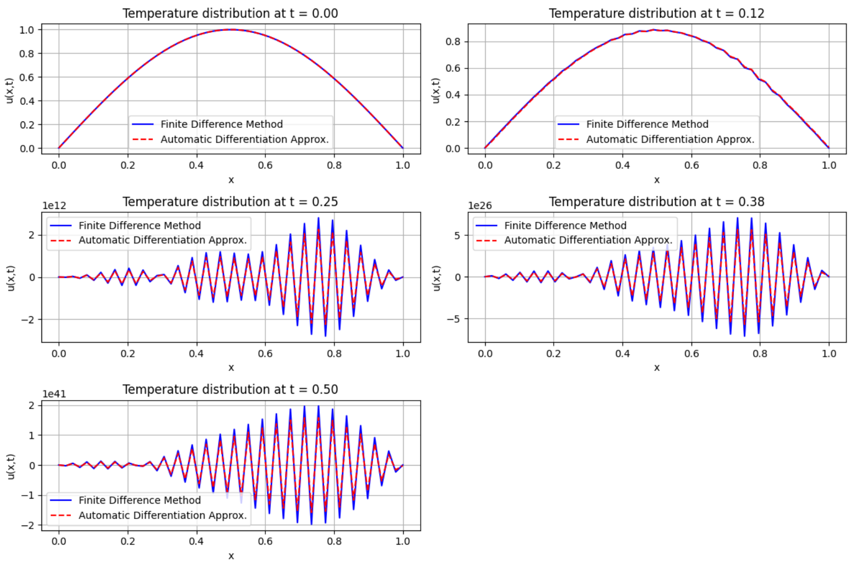

Figure 1. Comparison of temperature profiles obtained by grid-based and automatic differentiation methods

4. CONCLUSION

This study presents a comparative analysis of two numerical methods—automatic differentiation and the classical grid-based finite difference method—for solving the heat diffusion equation in plant tissues. The results demonstrate that automatic differentiation provides enhanced accuracy, improved solution stability, and allows for larger time steps without significant loss of precision. In contrast, the finite difference method remains advantageous due to its simplicity and computational efficiency, particularly when dealing with problems of lower complexity or with limited computational resources. These conclusions align well with recent developments in the field. For example, (Cai & Karniadakis 2021) show that physics-informed neural networks (PINNs), which utilize automatic differentiation, outperform traditional numerical techniques in solving heat transfer and multi-phase flow problems under uncertain and complex boundary conditions. Additionally, the multi-level PINN framework proposed by (He et al. 2023) highlights the practical viability of leveraging first- and second-order physical components separately, thereby increasing the stability and performance of neural solvers for higher-order differential systems. Furthermore, the integration of classical grid-based techniques with more flexible and adaptive neural solvers—as explored by (Ahmadi & Mohammadi 2022)—demonstrates the potential of hybrid schemes to combine the strengths of both methodologies. This study supports such a direction and suggests that hybrid numerical frameworks could offer improved modeling of nonlinear, anisotropic, and physiologically complex structures such as plant tissues. Future research should therefore focus on extending the current one-dimensional model to multi-dimensional formulations and include nonlinear effects such as anisotropic diffusion and metabolic dynamics. In addition, designing intelligent hybrid schemes that leverage both automatic differentiation and classical numerical stability can help further improve modeling precision and computational efficiency. Ultimately, this will contribute to a deeper understanding of the mechanisms underlying plant adaptation to extreme environmental conditions and expand the applicability of numerical methods in plant biophysics and related fields.

REFERENCES

Ahmadi, N., & Mohammadi, M. K. (2022). A hybrid differential transforms and finite difference method to numerical solution of convection–diffusion equation. *Applied Mathematics and Computation, 417*, 126748.

Baydin, A. G., Pearlmutter, B. A., Radul, A. A., & Siskind, J. M. (2018). Automatic differentiation in machine learning: A survey. *Journal of Machine Learning Research, 18*(153), 1–43.

Cai, S., Wang, Z., Wang, S., Perdikaris, P., & Karniadakis, G. E. (2021). Physics-informed neural networks (PINNs) for heat transfer problems. *Journal of Heat Transfer*, *143*(5), 050801.

Hajrulla, S., Uka, A., Ali, L., & Demir, T. (2023). Numerical methods and approximations for the heat transfer problem. *Proceedings of the International Conference on Academic Research in Science, Technology and Engineering, 1*(1), 21–31.

He, W., Li, J., Kong, X., & Deng, L. (2023). Multi-level physics-informed deep learning for solving partial differential equations in computational structural mechanics. *Computer Methods in Applied Mechanics and Engineering, 396*, 115220.

Morton, K. W., & Mayers, D. F. (2005). *Numerical solution of partial differential equations: An introduction* (2nd ed.). Cambridge University Press.

Patankar, S. V. (1980). *Numerical heat transfer and fluid flow*. Hemisphere Publishing Corporation.

Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics, 378*, 686–707.