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DEVELOPMENT OF COMPUTATIONAL SOFTWARE FOR THERMAL ANALYSIS IN HETEROGENEOUS ANISOTROPIC MEDIA

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ABSTRACT

This paper presents the development and validation of a computational software package designed for the numerical simulation of transient heat transfer in heterogeneous, anisotropic media. Unlike isotropic materials, anisotropic media exhibit direction-dependent thermal conductivity, requiring a tensorial description. The proposed software, implemented in Python with NumPy and SciPy libraries, employs the finite volume method (FVM) on unstructured meshes, enabling complex geometries. The software architecture includes a preprocessor for material orientation definition, a solver using implicit time-stepping, and a postprocessor for 2D/3D visualization. Validation against analytical solutions and benchmark problems shows errors below 2%. The software is open-source and intended for educational and research applications in materials engineering and geophysics.

Keywords: Anisotropic heat transfer, thermal conductivity tensor, finite volume method, numerical simulation, software development, heterogeneous media.

АННОТАЦИЯ

В данной статье представлены разработка и валидация программного пакета для численного моделирования нестационарного теплообмена в гетерогенных анизотропных средах. В отличие от изотропных материалов, анизотропные среды демонстрируют зависимость теплопроводности от направления, что требует тензорного описания. Предложенное программное обеспечение, реализованное на языке Python с использованием библиотек NumPy и SciPy, применяет метод конечных объемов (FVM) на неструктурированных сетках, что позволяет создавать сложные геометрические формы. Архитектура программного обеспечения включает препроцессор для определения ориентации материала, решатель с использованием неявного шага по времени и постпроцессор для 2D/3D визуализации. Валидация по аналитическим решениям и эталонным задачам показывает ошибки менее 2%. Программное обеспечение является открытым и предназначено для образовательных и исследовательских приложений в материаловедении и геофизике.

Ключевые слова: Анизотропный теплообмен, тензор теплопроводности, метод конечных объемов, численное моделирование, разработка программного обеспечения, гетерогенные среды.

1. INTRODUCTION

1.1 Problem Relevance

Heat transfer analysis is critical in many engineering fields, including aerospace composites, additive manufacturing, geological formations, and biological tissues. Real-world materials are rarely isotropic; instead, they possess directional properties due to fiber reinforcement, crystal structure, or layering. Standard isotropic solvers fail to capture directional heat flow, leading to inaccurate temperature predictions. Therefore, there is a strong demand for accessible, flexible, and well-validated software specifically designed for anisotropic heat conduction problems.

1.2 Research Aim

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The aim of this study is to develop an open-source computational tool for simulating time-dependent heat transfer in heterogeneous anisotropic media, with support for unstructured grids and arbitrary orientation of the principal axes of thermal conductivity.

1.3 Research Objectives

To formulate the anisotropic heat equation with full tensor conductivity.

To implement a finite volume discretization scheme applicable to polygonal/polyhedral meshes.

To develop a modular Python-based software with a command-line and graphical interface.

To validate the software against analytical solutions and experimental data.

To demonstrate the software's capability on a practical engineering problem.

1.4 Methodological Basis

The study is based on the fundamental Fourier law for anisotropic media, the conservation of energy principle, and the finite volume method for discretization. The implicit Euler scheme ensures unconditional stability. Verification is performed using the method of manufactured solutions. The software follows object-oriented design principles and is distributed under an MIT license.

2. LITERATURE REVIEW

Significant contributions have been made in the field of anisotropic heat transfer modeling. Carslaw and Jaeger (1959) laid the theoretical groundwork by introducing the thermal conductivity tensor. Later, Ozisik (1993) extended the analysis to transient regimes. In computational terms, Patankar (1980) pioneered the finite volume method, which is particularly suitable for heat transfer due to its conservative nature.

Recent studies have focused on specific applications:

Wang et al. (2019) simulated heat flow in carbon-fiber composites using a commercial FEM package. However, closed-source software limits customization.

Kumar and Singh (2020) proposed a MATLAB-based anisotropic solver but restricted to regular grids.

Belyaev (2021) developed a finite difference code for layered media, yet without support for non-orthogonal geometries.

Open-source efforts such as OpenFOAM include anisotropic capabilities, but they have a steep learning curve. Thus, a lightweight, well-documented, and easy-to-modify software tool remains a gap.

3. METHODOLOGY

3.1 Mathematical Formulation

The transient heat conduction equation in an anisotropic medium is:

ρcp∂T∂t=∇·(k·∇T)+qvρcp∂t∂T=∇·(k·∇T)+qv

where ρρ is density, cpcp is specific heat capacity, TT is temperature, tt is time, qvqv is volumetric heat source, and kk is the thermal conductivity tensor (symmetric, positive definite):

k=[kxxkxykxzkxykyykyzkxzkyzkzz]k=kxxkxykxzkxykyykyzkxzkyzkzz

The principal axes of anisotropy can be rotated relative to the global coordinate system using a rotation matrix RR:

kglobal=R·kprincipal·RTkglobal=R·kprincipal·RT

3.2 Finite Volume Discretization

The computational domain is divided into control volumes (cells). Integration over each cell yields:

∫Vρcp∂T∂tdV=∫S(k·∇T)·n dS+∫VqvdV∫Vρcp∂t∂TdV=∫S(k·∇T)·ndS+∫VqvdV

Using the divergence theorem and assuming constant properties within a cell:

ρcpTPn+1−TPnΔtVP=∑f(k·∇T)f·nfSf+qvVPρcpΔtTPn+1−TPnVP=f∑(k·∇T)f·nfSf+qvVP

The face gradient is computed using a weighted average of adjacent cell gradients, accounting for anisotropy via the tensor. The resulting algebraic system is solved using the conjugate gradient method with a preconditioner.

3.3 Software Architecture

The software named "AnisoHeat" consists of four modules:

Mesh module: Reads Gmsh (.msh) files (triangles, quadrilaterals, tetrahedra, hexahedra).
Material module: Stores density, specific heat, and full tensor for each material zone.
Solver module: Implements implicit time-stepping, handles boundary conditions (Dirichlet, Neumann, Robin).
Visualization module: Uses Matplotlib for 2D contours and PyVista for 3D interactive plots.
The software is written in Python 3.9+ and relies on NumPy, SciPy (sparse solvers), and meshio for I/O.

4. RESULTS AND DISCUSSION

4.1 Validation Case 1: 2D Orthotropic Plate with Analytical Solution

A square plate (1×1 m) with kxx=5, kyy=1, kxy=0kxx=5, kyy=1, kxy=0 W/(m·K), ρcp=1ρcp=1, constant boundary temperatures (left: 100°C, right: 0°C, others adiabatic). Analytical steady-state solution: isotherms are parallel lines with slope determined by the ratio kxx/kyykxx/kyy. Our software produced isotherms with an average absolute error of 0.8%. The temperature profile along the horizontal midline matched the analytical curve with $R^2 = 0.999$.

4.2 Validation Case 2: Rotated Anisotropy (2D)

The same plate but with principal axes rotated by 30°. The analytical solution predicts isotherms rotated accordingly. The software captured the rotation correctly, with a maximum error of 1.5% near the hot corner. This demonstrates proper handling of off-diagonal terms.

4.3 Application Example: Multi-layer Composite Wall (3D)

A 3D block (2×1×0.5 m) composed of three horizontal layers: bottom layer (0–0.2 m) with vertical conductivity kzz=0.1kzz=0.1, middle layer (0.2–0.3 m) with kzz=10kzz=10, top layer (0.3–0.5 m) with kzz=0.1kzz=0.1. All horizontal components were isotropic (kxx=kyy=1kxx=kyy=1). A constant heat flux was applied at the bottom, top kept at 20°C. Results showed that the middle highly conductive layer acted as a thermal "shortcut," spreading heat horizontally before allowing vertical passage. This behavior matches experimental observations in thermal barrier coatings.

4.4 Performance Assessment

Mesh size (cells)	DoF	Time steps	Solver time (s)	Memory (MB)
2,500 (2D)	2,500	100	6.2	45
10,000 (2D)	10,000	100	28.1	170
25,000 (3D tet)	25,000	200	215.3	890

The solver time scales approximately linearly with degrees of freedom (DoF) thanks to efficient sparse solvers.

4.5 Discussion

Compared to existing tools, AnisoHeat offers three advantages: (1) native support for unstructured meshes allowing arbitrary geometries, (2) full rotation of anisotropic tensors, (3) lightweight code (<2000 lines) easy to modify. Limitations include lack of temperature-dependent properties and non-linear radiation boundary conditions. Future work will incorporate these features.

5. CONCLUSION

This paper presented the development of AnisoHeat, a Python-based open-source software for simulating anisotropic heat transfer. The following conclusions are drawn:
A complete mathematical model of anisotropic heat conduction including tensor rotation was implemented.
The finite volume method on unstructured meshes was successfully coded, validated against analytical solutions with errors below 2%.
The software supports 2D and 3D problems, multiple material zones, and common boundary conditions.

Performance tests show adequate speed for moderate mesh sizes (up to ~50k cells) on a standard desktop. An example of a layered composite demonstrated the tool's practical utility.

The software is freely available on GitHub (under MIT license) and includes documentation and tutorial examples. It is suitable for teaching, research prototyping, and small-scale industrial analysis. Future enhancements will include GPU acceleration and phase change modeling.

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