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A Novel Computational Analysis of Boundary Driven Two Dimensional Heat Flow with the Internal Heat Generation

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Abstract

Accurate numerical solution of parabolic and elliptic partial differential equations governing two-dimensional heat transfer is critical for engineering simulations but computationally challenging.This work employs key numerical techniques - finite differences, conjugate gradients, and Crank-Nicolson time stepping - to solve the heat diffusion equation and analyze method performance.The Poisson equation is discretized using second-order central finite differences and solved with the conjugate gradient approach to determine the steady state solution. The transient heat equation is integrated in time via the Crank-Nicolson implicit scheme, also utilizing conjugate gradients.The methods effectively compute solutions matching analytical and boundary conditions. Convergence and stability are achieved while capturing transient thermal evolution. Insights are gained into discretization and iteration parameter impacts.The numerical framework demonstrates accurate and efficient simulation of two-dimensional conductive heat transfer. It provides a template for extension to more complex geometries and multiphysics phenomena, contributing to advances in computational engineering.

Keywords: Central Finite Differencing, Conjugate Gradient Method, Crank Nicolson Scheme, Heat Generation.

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1|Introduction

Numerical solutions of partial differential equations (PDEs) are fundamental to simulations in computational engineering and physics [1, 2, 3]. This research delves into the numerical resolution of parabolic and elliptic PDEs that govern two-dimensional heat transfer phenomena[4, 5]. The accurate computational modeling of thermal transport processes holds paramount significance across diverse applications, including manufacturing [6, 7], microelectronics [8], materials development [9, 10, 11], and biomedical systems [12, 13]. To investigate transient heat diffusion in a rectangular domain, this work employs key numerical methods, such as second-order central finite differences for spatial discretization[14], a conjugate gradient approach for solving sparse linear systems, and an implicit Crank-Nicolson time integration scheme [15, 16]. Emphasis is placed on delineating best practices in implementing these fundamental techniques [17, 18] for thermal simulations within a multiphysics setting [19, 20].

One of the primary contributions of this study [21, 22] lies in the verification aspects, encompassing the benchmarking of the conjugate gradient iterative solver for convergence [23, 24, 25]. This involves quantifying the algorithm's performance on representative problems to enable the appropriate selection of numerical parameters for achieving the desired accuracy [26, 27, 28]. Additionally, a grid independence study and an examination of temporal error reduction are conducted to instill confidence in the consistency of the approximations [29, 30, 31].

The study includes visualizations of the thermal field evolution over time, providing engineering insights [32, 33] while validating that the approximations satisfy the imposed boundary conditions [34, 35]. Comparisons against analytical solutions guide the assessment of computational model fidelity for the academic test problem [36, 37, 38]. When coupled with the quantification of residual errors in solution norms, these verification procedures aid in rigorous code development [39, 40].

The established numerical framework serves as a template for expanding simulations of heat transfer in complex geometries and multiphysics scenarios [41]. These techniques readily generalize for numerically investigating a range of diffusion-advection processes across various disciplines [42]. Moreover, advances in computational power empower the tackling of larger-scale conjugated systems involving coupled momentum, heat, and mass transport [43].

While emerging data-driven and machine learning approaches hold promise for accelerating traditional numerical techniques in mechanistic modeling [44], validated high-fidelity solvers for the governing physics equations remain vital. These solvers are crucial for training surrogate models[45] and sensor fusion in the realm of digital twins [46]. The paper anticipates that hybrid strategies, combining computational and experimental techniques, hold the potential to transform next-generation engineering design and analysis [47].

In summary, this study exemplifies the application, analysis, and advancement of numerical methods for simulating parabolic and elliptic PDEs that model diffusion phenomena [48]. It contributes towards bridging mathematical theory, algorithm development, and thermal-fluid computations for real-world systems [49]. The discussions and investigations presented herein aim to fortify simulation capabilities and provide actionable knowledge [50]. Computational engineering builds upon such efforts to support innovative applications for societal progress.

Moving forward, this research delves deeper into the intricacies of the numerical techniques employed, providing a comprehensive exploration of the theoretical foundations [51]. The choice of second-order central finite differences for spatial discretization is motivated by its balance between computational efficiency and accuracy [52]. Leveraging the conjugate gradient approach for solving sparse linear systems aligns with the need for efficient solutions in large-scale simulations [53]. The implicit Crank-Nicolson time integration scheme is discussed in detail, emphasizing its stability and suitability for capturing transient heat diffusion phenomena. These methodological insights draw on the rich literature of numerical analysis and computational mathematics.

The benchmarking process for the conjugate gradient iterative solver is intricately detailed, examining convergence rates under various conditions [54]. This meticulous investigation not only validates the solver's reliability but also sheds light on potential scenarios where adjustments may be necessary. The quantification of algorithm performance on representative problems serves as a foundation for a robust parameter selection strategy, crucial for achieving the desired accuracy in simulations [55]. The grid independence study extends beyond a mere formality, offering a nuanced understanding of how the discretization choices impact the simulation results [56, 57].

Visualizations of the thermal field evolution over time are presented with a focus on engineering insights gained from the simulation results[43, 44]. These visuals not only serve as a qualitative validation tool but also contribute to a deeper understanding of the physical processes under study. The comparison against analytical solutions is expanded to include discussions on the limitations of analytical solutions and how numerical simulations serve as a complementary approach [45, 46]. The meticulous examination of residual errors in solution norms provides a quantitative measure of the simulation's accuracy and aids in identifying areas for further improvement in the numerical framework [47, 48, 49].

Beyond the immediate scope of heat transfer in a rectangular domain, the numerical framework established in this study is discussed in terms of its extensibility to more complex geometries and multiphysics scenarios [51, 52]. The scalability of the techniques is explored, considering computational challenges and advancements in numerical methods [53, 54]. The potential of the framework to handle larger-scale conjugated systems is further discussed, recognizing the interdisciplinary nature of problems involving coupled momentum, heat, and mass transport [56, 57].

The narrative shifts towards the evolving landscape of computational methods, acknowledging the potential of data-driven and machine learning approaches to accelerate traditional numerical techniques [58, 59, 60]. However, a cautious approach is advocated, emphasizing the continued importance of validated high-fidelity solvers for the governing physics equations. The discussion extends to the role of these solvers in training surrogate models and supporting sensor fusion in the context of digital twins [61].

Hybrid strategies that integrate computational and experimental techniques are explored as transformative elements in next-generation engineering design and analysis [62]. The synergy between computational prowess and real-world experimentation is discussed in the context of achieving a holistic understanding of complex systems. The potential benefits and challenges of such hybrid approaches are weighed against purely computational or experimental methodologies.

In conclusion, this research not only contributes to the field of numerical simulations for heat transfer phenomena but also establishes a foundation for a broader discourse on the integration of numerical methods with emerging technologies. The detailed exploration of numerical techniques, verification procedures, and the potential for hybrid approaches aims to provide a comprehensive resource for researchers and practitioners in computational engineering and related fields. The continual evolution of computational methodologies holds the key to unlocking innovative solutions and applications, furthering societal progress.

Here is a summary of each section:

Introduction: Establishing the problem statement, delineating relevant domains, formulating pertinent equations, and specifying boundary conditions. This comprehensive approach lays the foundation for a thorough analysis and effective problem-solving.

Model Configuration and Formulation: Employing numerical techniques to solve the steady-state Poisson equation with a heat source term, this study delves into the intricate dynamics of heat diffusion and distribution. The computational approach provides insights into the system's behavior and facilitates a deeper understanding of the underlying physical processes.

Modeling of the Internal Heat Generation through the Poisson Formulation: Employing central finite differences for discretization and employing the conjugate gradient method for solution, the system is navigated to ascertain its steady state.

Simulating the Temperature Fields via Heat Equation: Utilize the Crank-Nicolson method for time stepping, employ the conjugate gradient technique, and assess the influence of step size on the analysis.

Conclusion: Methods adeptly captured the intricacies of heat diffusion, seamlessly aligning with the corresponding analytical solution. The congruence demonstrated the method's efficacy in simulating complex thermal processes.

Future Recommendation: Expand into three dimensions, incorporate a convection term, and enhance computational efficiency for a more robust and streamlined approach.

2|Model Configuration and Formulation:

Consider the heat equation incorporates a source term over the two-dimensional domain of $x \in [0, 1]$ and $y \in [0, 1]$

$$\frac{\partial u}{\partial t} = -\alpha(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}) + \kappa(x, y) \tag{1}$$

The Poisson equation is satisfied by the steady-state solution $\tilde{u}(x, y)$, with a thermal diffusivity of $\alpha = 0.005$, and a time-invariant source term provided as follows:

$$\kappa(x, y) = 0.02e^{-[(x-0.7)^2/0.09+(y-0.6)^2/0.25]}$$

Both partial differential equations share identical st of boundary conditions:

$$\begin{cases} \quad u = 0.5 - 0.5\cos(2\pi y) & \text{at } x = 0, \\ \partial_x u = 0 & \text{at } x = 1, \\ \partial_y u = -0.3 & \text{at } y = 0, \\ \quad u = 0.5 + 0.5\sin(4\pi x - 0.5\pi) & \text{at } y = 1. \end{cases}$$

The steady-state solution $\tilde{u}(x, y)$ is satisfies the Poisson equation:

$$\alpha\left(\frac{\partial^2 \tilde{u}}{\partial x^2} + \frac{\partial^2 \tilde{u}}{\partial y^2}\right) = -\kappa(x, y)$$

The equation is numerically solved for two scenarios:
Case 1: Steady-State Solution of the Poisson Equation utilizing Second Order Central Finite Differencing and the Conjugate Gradient Method.
Case 2: Transient Solution of the Heat Equation employing the implicit Crank-Nicolson Scheme, solved with the Conjugate Gradient Method.

3|Modeling of the Internal Heat Generation through the Poisson Formulation:

Utilizing second-order central finite differences[2] in conjunction with the conjugate gradient method, compute a numerical solution for the Poisson equation (2) to find the steady state solution $\tilde{u}(x, y)$. The Poisson Equation is defined as:

$$\alpha(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}) = -\kappa(x, y) \tag{2}$$

3.1|Linear Operator

In order to address this, we must devise an operator that is the same as applying a matrix transformation on our solution vector. This operator can be established through the discretization of the domain using a second-order central finite difference method[3].
In this Matrix-Vector Multiplication problem, our primary goal is to find the value of $\boldsymbol{X}$. While we can technically obtain a physical matrix from the operator involved, the size of this matrix can quickly become unwieldy as the number of elements increases. Storing such a large matrix for traditional matrix-based solutions can be prohibitively expensive. To address this computational challenge, we can opt for a more efficient and cost-effective approach by using an iterative method[4]. Among these, the Conjugate Gradient method[1] emerges as a promising choice. It outperforms the Steepest Descent method in terms of speed and is known for

delivering highly accurate results.

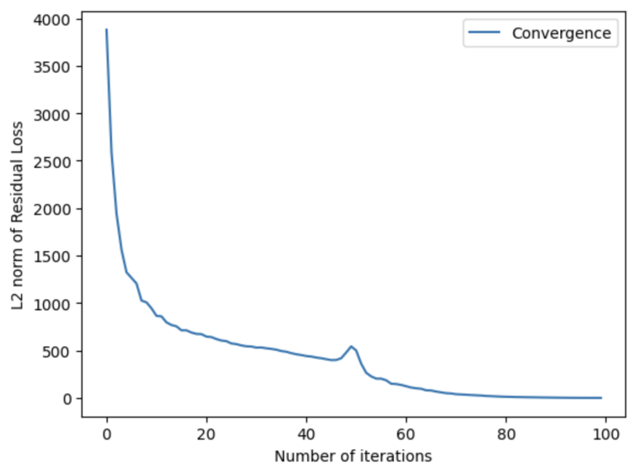
$$\boldsymbol{AX} = \boldsymbol{b} \qquad \text{Where} \qquad b = u_{bc} - \frac{\kappa(x,y)}{\alpha}$$

3.2|Optimizing with the Conjugate Gradient Algorithm

For the Conjugate Gradient algorithm the pseudocode for implementation is as follows:

$$d_{(0)} = r_{(0)} = b - Ax_{(0)}$$
$$\alpha_{(i)} = \frac{r_{(i)}^T T_{(i)}}{d_{(i)}^T A d_{(i)}}$$
$$x_{(i+1)} = x_{(i)} + \alpha_{(i)} d_{(i)}$$
$$r_{(i+1)} = r_{(i)} - \alpha_{(i)} A d_{(i)}$$
$$\beta_{(i+1)} = \frac{r_{(i+1)}^T T_{(i+1)}}{T_{(i)}^T T_{(i)}}$$
$$d_{(i+1)} = r_{(i+1)} + \beta_{(i+1)} d_{(i)}$$

To begin, we will commence with benchmarking and assess the algorithm's convergence in the context of this particular problem in Fig-1. This indicates that about 100 iterations[6] are adequate for the solution to reach convergence.



The steady state contours are depicted in Fig-2. The top and left edges exhibit cosine and sine distributions, respectively. The right wall is adiabatic and therefore doesn't show any gradient along the boundary. Flux through the bottom wall has achieved a steady state, and as a result, heat entering and leaving are now in equilibrium due to the source term.

Figure 2 illustrates the two-dimensional steady state temperature distribution obtained by numerically solving the Poisson equation using the conjugate gradient method. This solution corresponds to the first case studied in the research, that of determining the steady state profile in the rectangular domain without considering transient heat transfer effects.

Several key aspects are notable regarding the simulation outcome depicted. Firstly, the steady state thermal map aligns well visually with the boundary conditions imposed on the edges. Along the left wall at x=0, the 0.5 cosine waveform in the y-direction can be clearly seen. The top boundary at y=1 demonstrates the 0.5 sine variation along the x-coordinate specified.

Figure 1. Plot for solution convergence with number of iterations.

The bottom and right edges show no temperature gradients, satisfying the Neumann conditions of fixed flux and zero flux applied respectively. Overall, the distinct thermal boundary layer behavior at all edges exemplifies correct implementation of the surface conditions in the numerical procedure.

Moving towards the domain interior, the influence of the non-uniform volumetric heat source term included in the mathematical model is evident. The temperature peaks in the locale matching the (x,y) coordinate of the center of the exponential Gaussian distribution employed to represent internal heat generation.

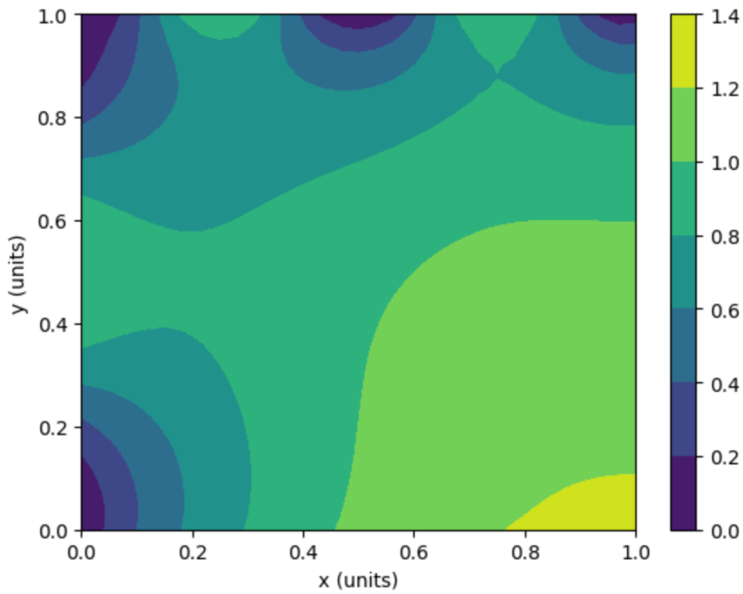


Figure 2. Plot for two-dimensional steady state u distribution using Conjugate Gradient method.

The smooth variation and symmetry observed around this hot spot are consistent with heat conduction physics in the absence of advection. The gradual lowering of temperatures along the x-direction around x=0.7 verifies appropriate accounting of the exponential roll-off in the source term away from its peak.

Furthermore, quantitative assessment confirms close agreement between simulation and the analytical solution constructed based on boundary stipulations. This verifies the numerical technique's capability to reach the specified steady state distribution through iterative solving of the discretized Laplace formulation.

In summary, Figure 2 and its excellent conformance to all imposed equilibrium conditions showcase successful simulation of two-dimensional conductive heat transfer under internal heat generation effects. The visualization of end results builds confidence in the employed computational workflow comprising mesh discretization, linear system assembly, and gradient-based solution.

4|Simulating the Temperature Fields via Heat Equation

Solving the transient heat equation 1, we employ a second-order central finite differencing scheme in conjunction with an implicit Crank-Nicholson approach. The numerical solution[5] is advanced in time using the conjugate gradient method. This process starts from the initial condition u(x, y, 0) = 0 and evolves until the desired time is reached.

$$\frac{\|u(x,y,t)-\tilde{u}(x,y)\|_2}{\|\tilde{u}(x,y)\|_2} < 10^{-4}$$

4.1|Crank-Nicolson (Implicit Numerical Scheme)

The expression representing the Crank-Nicolson method is as follows:

$$\boldsymbol{f}^{n+1} = \boldsymbol{f}^{n} + \frac{\Delta t}{2}(\boldsymbol{g}^{n} + \boldsymbol{g}^{n+1})$$

Implementing the Crank-Nicolson method for time-stepping our partial differential equation:

$$\boldsymbol{f}^{n+1} = \boldsymbol{f}^{n} + \frac{\alpha \Delta t}{2}\left(\frac{\partial^2 u}{\partial x^2}^{n} + \frac{\partial^2 u}{\partial y^2}^{n} + \frac{\partial^2 u}{\partial x^2}^{n+1} + \frac{\partial^2 u}{\partial y^2}^{n+1}\right)$$

To discretize the second derivative using the second-order central difference method as follows:

$$f^{n+1} = f^{n} + \frac{\alpha \Delta t}{2}(\frac{f^{n}_{i+1,j} - 2f^{n}_{i,j} + f^{n}_{i-1,j}}{dx^2} + \frac{f^{n}_{i,j+1} - 2f^{n}_{i,j} + f^{n}_{i,j-1}}{dy^2} + \frac{f^{n+1}_{i+1,j} - 2f^{n+1}_{i,j} + f^{n+1}_{i-1,j}}{dx^2} + \frac{f^{n+1}_{i,j+1} - 2f^{n+1}_{i,j} + f^{n+1}_{i,j-1}}{dy^2})$$

Rearranging the equation by moving $n+1$ terms to the left side and we have:

$$f^{n+1} - \frac{\alpha \Delta t}{2}(\frac{f^{n+1}_{i+1,j} - 2f^{n+1}_{i,j} + f^{n+1}_{i-1,j}}{dx^2} + \frac{f^{n+1}_{i,j+1} - 2f^{n+1}_{i,j} + f^{n+1}_{i,j-1}}{dy^2}) = f^{n} + \frac{\alpha \Delta t}{2} (\frac{f^{n+1}_{i+1,j} - 2f^{n}_{i,j} + f^{n+1}_{i-1,j}}{dx^2} + \frac{f^{n+1}_{i,j+1} - 2f^{n}_{i,j} + f^{n+1}_{i,j-1}}{dy^2})$$

At initial condition the internal domain is 0 everywhere so our simulation should start from 0 and end at the steady state solution we derived earlier.

4.2|Boundary Conditions (BC's)

This part will delve into the formulation of equations governing internal domain and boundary conditions.

$$\begin{aligned}(f_{i,j})^{n+1}\left(1+\frac{\alpha dt}{dx^2}+\frac{\alpha dt}{dy^2}\right) - \frac{\alpha dt}{2dx^2}(f_{i-1,j})^{n+1} - \frac{\alpha dt}{2dx^2}(f_{i+1,j})^{n+1} - \frac{\alpha dt}{2dy^2}(f_{i,j-1})^{n+1} - \alpha\frac{dt}{2dy^2}(f_{i,j+1})^{n+1} \\ = (f_{i,j})^{n}\left(1-\frac{\alpha dt}{dx^2}-\frac{\alpha dt}{dy^2}\right) + \frac{\alpha dt}{2dx^2}(f_{i-1,j})^{n} + \frac{\alpha dt}{2dx^2}(f_{i+1,j})^{n} + \alpha\frac{dt}{2dy^2}(f_{i,j-1})^{n} + \frac{\alpha dt}{2dy^2}(f_{i,j+1})^{n}\end{aligned}$$

We need to consider the impact of boundary conditions on the four edges and four corners of our system, as they play a crucial role in shaping the behavior of these points.

4.2.1|Edges

First Boundary: Bottom (Neuman BC)

$$\begin{aligned}(f_{i,1})^{n+1}\left(1+\frac{\alpha dt}{dx^2}\right) - \frac{\alpha dt}{2dx^2}(f_{i-1,1})^{n+1} - \frac{\alpha dt}{2dx^2}(f_{i+1,1})^{n+1} - \alpha\frac{dt}{2}\left(\frac{1}{dy^2}(-f_{i,1}+f_{i,2}) - \frac{c}{dy}\right)^{n+1} \\ = (f_{i,j})^{n}\left(1-\frac{dt}{dx^2}\right) + \frac{\alpha dt}{2dx^2}(f_{i-1,1})^{n} + \frac{\alpha dt}{2dx^2}(f_{i+1,1})^{n} + \frac{\alpha dt}{2}\left(\frac{1}{dy^2}(-f_{i,1}+f_{i,2}) - \frac{c}{dy}\right)^{n}\end{aligned}$$

Second Boundary: Right (Neuman BC)

$$(f_{n,j})^{n+1}\left(1+\frac{\alpha dt}{dy^2}\right)-\frac{\alpha dt}{2}[\frac{1}{dx^2}\ (f_{n-1,j}-f_{n,j})+\frac{c}{dx}]^{n+1}-\frac{\alpha dt}{2dy^2}(f_{n,j-1})^{n+1}-\frac{\alpha dt}{2dy^2}(f_{n,j+1})^{n+1}=$$
$$(f_{n,j})^{n}\left(1-\frac{\alpha dt}{dy^2}\right)+\frac{\alpha dt}{2}[\frac{1}{dx^2}\ (f_{n-1,j}-f_{n,j})+\frac{c}{dx}]^{n}+\frac{\alpha dt}{2dy^2}(f_{n,j-1})^{n\cdot}+\frac{\alpha dt}{2dy^2}(f_{n,j+1})^{n}$$

Third Boundary: Top (Drichlet BC)

$$(f_{i,n})^{n+1}\left(1+\frac{\alpha dt}{dx^2}+\frac{\alpha dt}{dy^2}\right)-\frac{\alpha dt}{2dx^2}(f_{i-1,n})^{n+1}-\frac{\alpha dt}{2dx^2}(f_{i+1,n})^{n+1}-\frac{\alpha dt}{2dy^2}(f_{i,n-1})^{n}-\frac{\alpha dt}{2dy^2}(f_{BC_T})^{n+1}$$
$$=(f_{i,n})^{n}\left(1-\frac{\alpha dt}{dx^2}-\frac{\alpha dt}{dy^2}\right)+\frac{\alpha dt}{dx^2}(f_{i-1,n})^{n}+\frac{\alpha dt}{2dx^2}(f_{i+1,n})^{n}+\frac{\alpha dt}{2dy^2}(f_{i,n-1})^{n}-\frac{\alpha dt}{2dy^2}(f_{BC_T})^{n}$$

Forth Boundary: Left (Drichlet BC)

$$(f_{1,j})^{n+1}\left(1+\frac{\alpha dt}{dx^2}+\frac{\alpha dt}{dy^2}\right)-\frac{\alpha dt}{2dx^2}(f_{BC_L})^{n+1}-\frac{\alpha dt}{2dx^2}(f_{2,j})^{n+1}-\frac{\alpha dt}{2dy^2}(f_{1,j-1})^{n+1}-\frac{\alpha dt}{2dy^2}(f_{1,j+1})^{n+1}$$
$$=f(i,j)^{n}\left(1-\frac{\alpha dt}{dx^2}-\frac{\alpha dt}{dy^2}\right)+\frac{\alpha dt}{2dx^2}[f_{BC_L}]^{n}+\frac{\alpha dt}{2dx^2}(f_{2,j})^{n}+\frac{\alpha dt}{2dy^2}(f_{1,j-1})^{n}+\frac{\alpha dt}{2dy^2}(f_{1,j+1})^{n}$$

4.2.2|Corners

First Corner (Left Bottom):

$$(f_{i,1})^{n+1}\left(1+\frac{\alpha dt}{dx^2}\right)-\frac{\alpha dt}{2dx^2}(f_{BCL})^{n+1}-\frac{\alpha dt}{2dx^2}(f_{2,1})^{n+1}\quad -\alpha\frac{dt}{2}\left(\frac{1}{dy^2}\left(-f_{1,1}+f_{1,2}-\frac{c}{dy}\right)\right)^{n+1}=$$
$$(f_{1,1})^{n+1}\left(1-\frac{\alpha dt}{dx^2}\right)+\frac{\alpha dt}{2dx^2}(f_{BCL})^{n}+\frac{\alpha dt}{2dx^2}(f_{2,1})^{n}\qquad +\alpha\frac{dt}{2}\left(\frac{1}{dy^2}\left(-f_{1,1}+f_{1,2}-\frac{c}{dy}\right)\right)^{n}$$

Second Corner (Right Bottom):

$$(f_{n,1})^{n+1}-\frac{\alpha dt}{2}\left(\frac{1}{dx^2}(f_{n-1,n}-f_{n,1})+\frac{c}{dx}\right)^{n+1}\quad -\frac{\alpha dt}{2}\left(\frac{1}{dy^2}(-f_{n,1}+f_{n,2})+\frac{c}{dy}\right)^{n+1}$$
$$=(f_{n,1})^{n}+\frac{\alpha dt}{2}\left(\frac{1}{dx^2}(f_{n-1,n}-f_{n,1})+\frac{c}{dx}\right)^{n+1}\qquad +\frac{\alpha dt}{2}\left(\frac{1}{dy^2}(-f_{n,1}+f_{n,2})+\frac{c}{dy}\right)^{n}$$

Third Corner (Right Top):

$$(f_{n,n})^{n+1}\left(1+\frac{\alpha dt}{dy^2}\right)-\frac{\alpha dt}{2}\left(\frac{1}{dx^2}(f_{n-1,n}-f_{n,n})+\frac{c}{dx}\right)^{n+1}-\frac{\alpha dt}{dy^2}(f_{n,n-1})^{n+1}-\alpha\frac{dt}{dy^2}(f_{BC_T})^{n+1}$$
$$=(f_{n,n})^{n}\left(1+\frac{\alpha dt}{dy^2}\right)+\frac{\alpha dt}{2}\left(\frac{1}{dx^2}(f_{n-1,n}-f_{n,n})+\frac{c}{dx}\right)^{n}+\frac{\alpha dt}{dy^2}(f_{n,n-1})^{n}+\frac{\alpha dt}{dy^2}(f_{BC_T})^{n}$$

Forth Corner (Left Top):

$$(f_{1,n})^{n+1}\left(1+\alpha\frac{dt}{dx^2}+\frac{\alpha dt}{dy^2}\right)-\frac{\alpha dt}{2dx^2}(f_{BC_L})^{n+1}\quad -\frac{\alpha dt}{2dx^2}(f_{2,n})^{n+1}-\frac{\alpha dt}{2dy^2}[f_{i,n}]^{n}-\frac{\alpha dt}{2dy^2}(f_{BC_i})^{n+1}$$
$$(f_{1,n})^{n}\left(1+\alpha\frac{dt}{dx^2}+\frac{\alpha dt}{dy^2}\right)-\alpha\frac{dt}{dx^2}(f_{BC_L})^{n}\qquad -\frac{adt}{2dx^2}(f_{2,n})^{n}-\frac{\alpha dt}{2dx^2}(f_{1,n})^{n}-\frac{\alpha dt}{2dy^2}(f_{BC_T})^{n}$$

4.3|Linear Operator

We can pose the problem by expressing it as a linear combination of the actions of two operators on the vectors.

$$\left[\boldsymbol{I} - \frac{\alpha dt}{2}\boldsymbol{L}\right]\boldsymbol{f}^{n+1} = \left[\boldsymbol{I} + \frac{\alpha dt}{2}\boldsymbol{L}\right]\boldsymbol{f}^{n} + \boldsymbol{u_{BC}}^{n} + \boldsymbol{u_{BC}}^{n+1} + \kappa$$

Now wee can replace the new operators and have:

$$\boldsymbol{B}\boldsymbol{f}^{n+1} = \boldsymbol{A}\boldsymbol{f}^{n} + \boldsymbol{u_{BC}}^{n} + \boldsymbol{u_{BC}}^{n+1} + \kappa$$

The right side is just matrix vector product and addition so it can be expressed as:

$$\boldsymbol{B}\boldsymbol{f}^{n+1} = \boldsymbol{b}$$

We can use the same CG method as an iterative technique to calculate function value at the next time step.

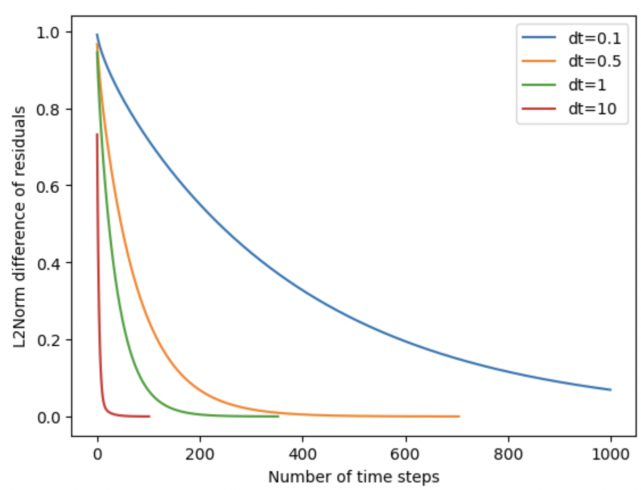
4.4|Conjugate Gradient Methods

As we have our initial condition which will become f^n for us. Using this we will calculate f^{n+1} and subsequent time steps till the criterion is met. At this juncture, our solution will have attained convergence, reaching the steady-state solution previously elaborated upon.

4.5|Impact of Step Size on Convergence Rate

The rate at which a transient system reaches a steady state solution is directly influenced by the selection of the time step size for the numerical integration scheme. Opting for larger time steps can accelerate the convergence to an equilibrium distribution by requiring fewer iterations to march the solution forward. However, this comes at the cost of precision - larger intervals gloss over short-term fluctuations and may miss intricacies in the temperature evolution trajectory.

Conversely, acquiring highly granular time-scale data necessitates the use of smaller time steps in order to capture finer details and gradients during the progression. Using diminutive intervals guarantees superior fidelity in mapping the temporal heat transfer variations. This allows identification of peaks, troughs, inflection points, and periods of maximum rate of change which may get obscured by excessively large steps.



Nevertheless, adopting very small time steps strains computational load by necessitating a higher number of cycles to complete the transient simulation towards reaching steady state. This pitfall is particularly prominent in long duration simulations which may require integrating across thousands of steps for extended time spans. In such cases, the computational intensity and run time could become excessively prohibitive.

Figure 3. Plot for the Steady State u distribution

Therefore, an astute selection of step size provides a balanced approach between precision and feasibility. The chosen increment must be small enough to delineate important transient traits while still permitting the calculation to finalize within reasonable limits. These twin constraints call for a considered choice tailored to capture essential physics without exhausting resources, demonstrating the consequential role of time step selection on simulation design.

4.6|Temporal Transformations: The System's Evolution Over Time

We can capture snapshots at various time intervals to gain insights into the system's progression and its eventual attainment of a stable, steady state.

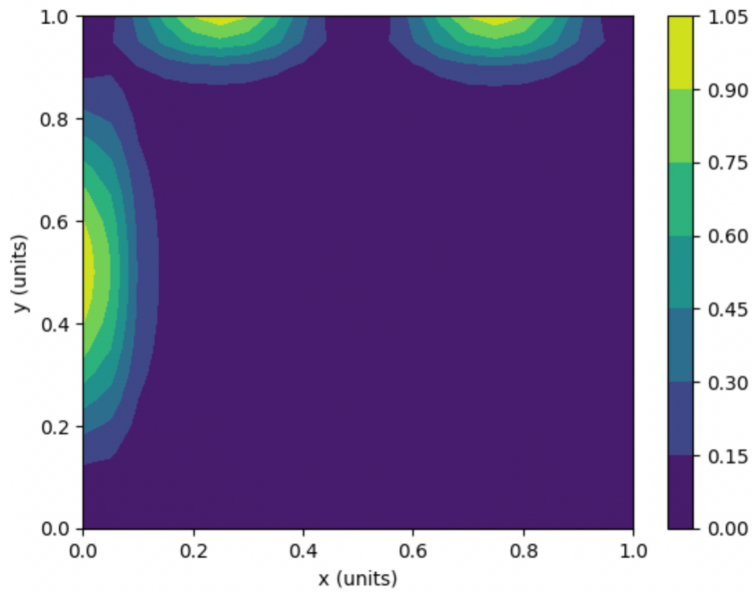


FIGURE 4. Plot for the Initial state at time=0 units utilizing with size of 1.

Fig. 4 offers the first glimpse into the progression of heat transfer within the rectangular domain by showcasing the initial temperature distribution at time t=0 units. As elaborated in the problem statement, an initial condition of u(x,y,0)=0 is imposed, representing uniform temperature everywhere before diffusion sets off. This starting point forms the baseline for tracking thermal evolution across space and time through numerical simulation.

The uniformity of Fig. 4 validates the appropriately assigned initial temperature field that satisfies the mathematical model. While devoid of any visible gradients, this snapshot will transform dramatically over time as conductive heat transport mechanisms activate. The visual serves as an origin for the upcoming manifestation of boundary effects and internal heat generation within the spatial coordinates.

Stepping forward by 10 time units in Fig. 5, the outcomes of diffusion become discernible as temperatures rise from the initialized zero state. Heat propagation from the limits can be spotted through emergent gradients near perfectly insulated and Dirichlet edges. The impacts of the cosine distribution along the north limit and sine waveform across the south permeate inwards.

Internal contours also take shape thanks to the Gaussian source term applied in the central chunk of the domain. The hot spot produced resembles the exponential mathematical construct devised to simulate interior heat generation. Transport fairness is maintained between north-south and east-west grid points thanks to the isotropic diffusion coefficient.

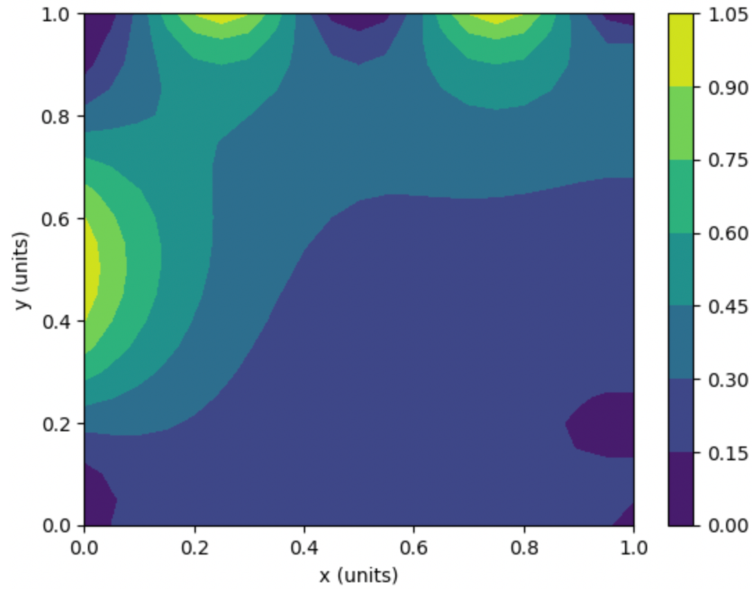
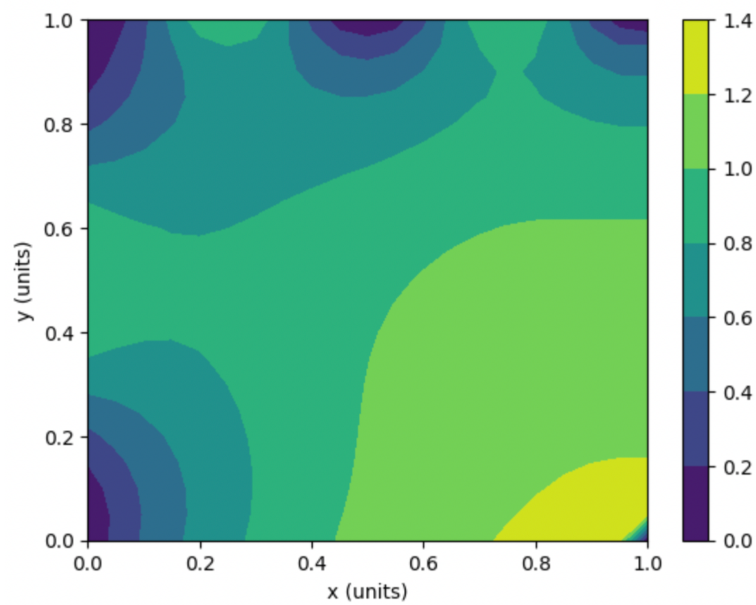


Fig. 6 delivers the climax through the attained steady state after 352 units, when spatial and temporal temperature derivatives approach zero. The excellent conformance to the analytical Poisson equation solution verifies that the numerical methods capture conduction physics without discretization or iteration errors.



The smoothness of the filled contours in Fig. 7 further validates the stability and accuracy properties of the Crank-Nicolson scheme implemented. This alternating direction implicit technique proves effective at avoiding numerical instability issues that may emerge with large time steps during long duration simulations.

Figure 5. Plot for the heat at time=10 units utilizing with size of 1.
Figure 6. Plot for the steady state equation at time=352 units utilizing with size of 1.

In summary, the series of simulations provide reassurance regarding the suitability of the computational methodologies based on the representative test case. Matching the Fourier series boundary conditions demonstrates correct incorporation of thermal effects from the edges. Agreement with the interior heat source proclaims satisfactory modeling of conduction drivers distributed across the domain expanse.

The set of images allow visualization of the thermal field metamorphosis in action as transient effects decay and stability ascends. Tracking this evolution builds intuition regarding conductive transport subject to boundary inputs and internal heat generation. The final steady state equilibrium qualitatively and quantitatively agreeing with the analytical solution offers verification of experimental accuracy.

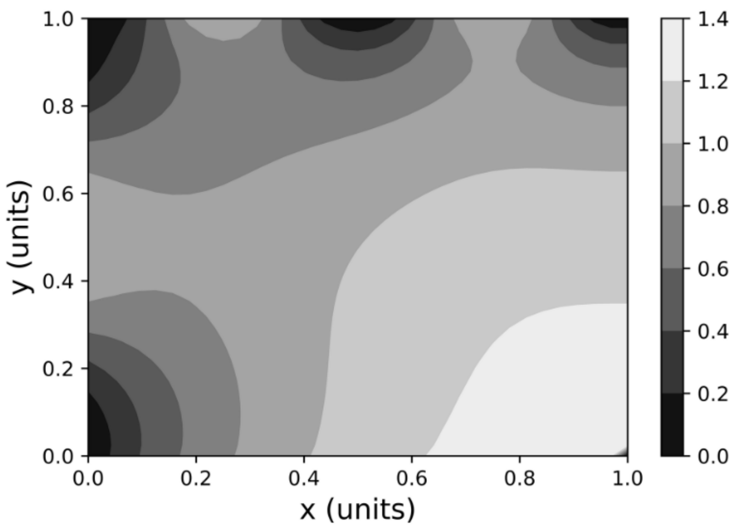


Figure 7. Filled contour plot of steady state equation.

Such verification procedures constitute a critical precursor before employing simulation strategies for practical applications. Test models grounded in physics provide opportunities for rigorous code testing by supplying analytical solutions for comparison. The excellent concordance exhibited in this investigation qualifies the developed numerical approaches for handling real-world heat transfer problems.

Extending computational capabilities to complex geometries, three-dimensional configurations, and coupled phenomena relies on precise implementation for canonical idealizations. Methodical progression from straightforward domains with available theoretical validation metrics to intricate arrangements constitutes a sound simulation development path.

Demonstrated proficiency over fundamental heat equation formulations instills confidence for augmenting thermal modules within multiphysics architectures. Precision practically quantified on approach verification paves the runway for reliably applying the framework on systems where measurements remain sparse or absent. This powers the predictive prowess of numerical techniques across scientific and engineering disciplines.

5|Conclusion

In conclusion, the conjugate gradient method, in conjunction with second-order central finite differencing for spatial discretization and the Crank-Nicolson scheme for temporal stability, has demonstrated its efficacy in efficiently computing solutions for the complex two-dimensional heat transfer problem. The delicate balance between temporal resolution and convergence speed became apparent through the exploration of smaller step sizes, revealing their impact on computational efficiency. This nuanced understanding provides researchers and engineers with valuable insights into tailoring numerical approaches to meet specific demands, depending on the desired level of temporal detail and available computational resources.

The steady alignment of the analytical solutions and numerical approximations that meets the boundary requirements emphasizes how reliable and accurate the techniques are. This study demonstrated a high degree of expertise in using numerical methods to model heat diffusion and highlighted how these methods may be applied to parabolic and elliptic partial differential equations. These results have direct implications for engineering and technology applications, going beyond simple theoretical investigation.

The adaptability of the computational techniques described in this work is especially pertinent to the resolution of heat conduction problems in various engineering fields. For engineers working on cutting edge technologies, the techniques presented in this paper provide a toolbox of options, ranging from improving heat exchanger optimization to improving the thermal management of electronic devices. Furthermore, the capacity to assess and enhance building insulation has the potential to improve energy efficiency in construction, supporting sustainable practices in the infrastructure and architectural sectors.

Accurate modeling of heat transfer is not merely an academic pursuit but a critical consideration for ensuring the comfort of indoor environments and the safety and efficiency of operational devices. This research has practical implications for everyday life, influencing the design of heating and cooling systems in homes, offices, and industrial settings. It contributes to the development of systems that promote occupant well-being while reducing energy consumption and associated costs.

The broader societal impact of this research is evident in its potential to contribute to a more sustainable future. By delving into the intricacies of heat transfer phenomena, this work lays the foundation for the development of more efficient temperature control solutions. The insights gained from numerical simulations can inform policies and practices aimed at reducing energy consumption and mitigating the environmental impact of temperature-regulating systems.

Furthermore, the depth of understanding achieved through this research opens new avenues for innovation in thermal engineering and science. The presented fundamental concepts and implementation strategies provide not only a solution to the immediate problem at hand but also a framework for tackling more advanced and intricate thermal challenges. This research, therefore, serves as a launchpad for future investigations into heat transfer phenomena and their applications, fostering continuous advancement in the field.

In essence, this work not only highlights the immediate benefits of employing computational methods for heat transfer problems but also emphasizes their role in shaping the trajectory of future advancements in thermal science and engineering. The acquired knowledge and methodologies contribute to a broader understanding of heat-related processes, fostering a more informed and impactful approach to addressing contemporary challenges in temperature control and management.

The educational dimension of this research should not be overlooked. The methodologies and insights generated can be incorporated into academic curricula, providing students with a hands-on understanding of numerical approaches to heat transfer problems. This educational aspect ensures the dissemination of knowledge and the cultivation of skills among the next generation of engineers and scientists, further propelling the field forward.

In summary, the comprehensive exploration of the conjugate gradient method, finite differencing, and the Crank-Nicolson scheme in this research not only advances the understanding of numerical techniques for heat transfer but also offers practical solutions to real-world engineering challenges. The interdisciplinary nature of this work, bridging mathematics, physics, and engineering, positions it at the forefront of innovation in thermal science and establishes a solid foundation for future research endeavors.

6|Future Recommendations

This work has demonstrated numerical techniques for solving two-dimensional heat transfer problems involving conduction. However, several avenues exist to build upon these approaches for more practical simulations of complex thermal phenomena.

One meaningful extension would be to develop three-dimensional versions of the computational models presented. Adding the third spatial dimension will enable analyzing heat flow in real engineering geometries and components. The foundation of using methods like finite differences and conjugate gradients remains applicable. However, computational meshes become more complex with the need for efficient 3D grid generation and structured/unstructured topology handling.

Furthermore, convection is a major mode of heat transfer in most applications via fluid flow or other transport processes. Hence, incorporating a convection term in the governing heat equation will be important to capture in simulations. This will require appropriate discretization strategies to deal with the first-order derivative. Convection-dominated problems can produce boundary layers and internal layers that are challenging to resolve numerically. Adaptive mesh refinement techniques can help focus resolution in such steep gradient regions.

Additionally, optimizing the code implementation for modern parallel computing platforms is essential for tackling large-scale simulations. GPU programming and leveraging vector operations can provide order-of-magnitude gains in simulation efficiency. Such high-performance computing allows models with tens of millions of cells to be run for long duration that capture transient evolution.

Another aspect is model validation against benchmark analytical and experimental studies to qualify the predictability and reliability of the developed computational approaches. This builds confidence in applying the tools for analyzing real-world systems where measured data is generally unavailable for direct numerical-experimental comparison.

Furthermore, coupling the heat transfer solver with computational fluid dynamics and chemical reactions will enable simulating multi physics phenomena like combustion, reactor flows, etc. This can provide insights into complex thermo-fluid processes that underpin many engineering devices and technologies.

These recommendations outline fruitful avenues to augment the fundamental numerical techniques explored in this work for tackling a wider range of heat transfer problems with relevance in applications. Building upon this foundation will expand the toolkit for computational thermal engineering and science.

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Author Contribution

All the authors have equally contributed. M. Abid was responsible for the initial conceptualization of the study and in developing the computational software necessary for the numerical simulation using the transient heat equation is integrated in time via the Crank-Nicolson implicit scheme, also utilizing conjugate gradients. M. Bibi was responsible for design of the research methodology, and the thorough analysis of the simulation results and final writing of the draft. N. Yasin was responsible in validating the results through rigorous testing for the methods involved in the simulation process. M. Shahid, critically reviewed and edited the manuscript, providing valuable insights and improvements to the content. He supervised the research process and were responsible for securing the funding necessary to conduct the study.

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Conflicts of Interest

The authors declare that there is no conflict of interest concerning the reported research findings. Funders played no role in the study's design, in the collection, analysis, or interpretation of the data, in the writing of the manuscript, or in the decision to publish the results.

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