

A STABILITY-ADMISSIBLE OPTIMIZATION FRAMEWORK FOR TIME-STEP SELECTION IN FINITE DIFFERENCE HEAT EQUATION SOLVERS

*(Kerangka Pengoptimuman Berasaskan Kestabilan untuk Pemilihan Langkah Masa dalam
Penyelesaian Persamaan Haba Kaedah Perbezaan Terhingga)*

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ABSTRACT

The one-dimensional heat equation is a fundamental parabolic partial differential equation used to model diffusive heat transfer processes. Although classical finite difference schemes are well established, their numerical accuracy depends on the selected time-step size. In practice, the time step is often chosen using stability restrictions such as the Courant–Friedrichs–Lewy (CFL) condition. However, stability does not necessarily correspond to minimum numerical error. Therefore, this study formulates the time-step selection problem as a constrained optimization problem within the stability-admissible region. The objective function is defined using the discrete maximum error between the numerical and exact solutions at the final simulation time. First, the time-step selection problem is formulated as a constrained optimization problem under the stability condition. Second, the numerical error is evaluated through the maximum norm of the difference between the numerical and exact solutions. Third, Particle Swarm Optimization (PSO) is used to determine suitable time-step values automatically. Since the optimization problem is bounded and nonlinear, PSO provides a simple derivative-free search strategy without requiring gradient information. Numerical results for the FTCS and Crank–Nicolson schemes show that different time-step values produce noticeably different numerical errors. Then, the optimization procedure consistently identifies time-step values with smaller error than conventional manually selected parameters. The results suggest that satisfying stability conditions alone is insufficient to obtain accurate numerical solutions.

Keywords: heat equation; finite difference method; metaheuristics optimization

ABSTRAK

Persamaan haba satu dimensi merupakan persamaan pembezaan separa parabola asas yang digunakan untuk memodelkan proses pemindahan haba resapan. Walaupun skema beza terhingga klasik telah lama digunakan, ketepatan numeriknya bergantung pada pemilihan saiz langkah masa yang digunakan. Langkah masa lazimnya dipilih berdasarkan kekangan kestabilan seperti syarat Courant–Friedrichs–Lewy (CFL). Walau bagaimanapun, kestabilan tidak semestinya menghasilkan ralat numerik minimum. Oleh itu, kajian ini memformulasikan masalah pemilihan langkah masa sebagai masalah pengoptimuman terkekang dalam rantau yang memenuhi syarat kestabilan. Fungsi objektif ditakrifkan menggunakan ralat maksimum diskret antara penyelesaian numerik dan penyelesaian tepat pada masa simulasi akhir. Pertama, masalah pemilihan langkah masa diformulasikan sebagai masalah pengoptimuman terkekang di bawah syarat kestabilan. Kedua, ralat numerik dinilai menggunakan norma maksimum bagi perbezaan antara penyelesaian numerik dan penyelesaian tepat. Ketiga, Pengoptimuman Kawanan Zarah (Particle Swarm Optimization, PSO) digunakan untuk menentukan nilai langkah masa yang sesuai secara automatik. Oleh sebab masalah pengoptimuman tersebut bersifat terkekang dan tidak linear, PSO menyediakan strategi carian mudah tanpa terbitan dan tidak memerlukan maklumat kecerunan. Keputusan numerik bagi skema FTCS dan Crank–Nicolson menunjukkan bahawa nilai langkah masa yang berbeza menghasilkan ralat numerik yang ketara berbeza. Seterusnya, prosedur pengoptimuman secara konsisten mengenal pasti nilai langkah masa yang

menghasilkan ralat lebih kecil berbanding parameter yang dipilih secara manual menggunakan pendekatan konvensional. Keputusan kajian menunjukkan bahawa pematuhan terhadap syarat kestabilan sahaja tidak mencukupi untuk memperoleh penyelesaian numerik yang tepat.

Kata kunci: persamaan haba; kaedah perbezaan terhingga; pengoptimuman metaheuristik

1. Introduction

The one-dimensional heat equation is a fundamental parabolic partial differential equation that models transient heat conduction and diffusion processes. It serves as a standard benchmark in numerical analysis and applied mathematics. Its applications extend to thermal engineering (Mevawalla *et al.* 2021), material processing (Érchehyi & Rácz 2025), and diffusion-driven physical systems (Kalinay 2025). Although analytical solutions exist for several simplified cases, practical problems often involve transient dynamics and discretized spatial domains that prevent closed-form representations (Bağlan & Aslan 2024). Therefore, numerical methods are commonly used to approximate the solution of the heat equation. Among the available numerical approaches, finite difference methods are adopted due to their relatively simple formulation and direct discretization structure (Teixeira *et al.* 2023). However, their numerical performance is highly sensitive to discretization parameters, especially the time-step size. Improper parameter selection may result in numerical instability (Robertsson & Blanch 2021), large approximation error (Hajrulla *et al.* 2023), or unnecessary computational cost (Zhou *et al.* 2023). In practical simulations, smaller time steps generally improve accuracy but require more iterations, whereas larger time steps reduce computational effort but may produce noticeable numerical error. This trade-off highlights the limitation of stability-based parameter selection to ensure the validity of the solution. Classical stability analysis provides conditions that restrict the allowable time-step size, but these bounds do not guarantee optimal accuracy.

Recent studies in heat transfer problems have continued to highlight the importance of stability considerations in numerical simulations. For example, hybrid nanofluid flow models have shown that parameters such as suction strength, wedge angle, and magnetic effects can significantly influence the resulting thermal behaviour and solution structure (Zainal *et al.* 2025; 2021). Similar observations were reported in radiative heat transfer models involving non-Newtonian fluids, where the existence of multiple solution branches requires additional stability analysis to determine physically meaningful solutions (Waini *et al.* 2022; 2023). Although these studies focus on fluid flow and heat transfer applications, they demonstrate that parameter selection and stability analysis remain important aspects of reliable numerical computation.

The Forward Time Central Space (FTCS) method and the Crank–Nicolson method are two classical finite difference schemes that will be discussed in this study. For explicit schemes such as the Forward Time Central Space (FTCS) method, the time step must satisfy a stability condition to prevent divergence of the numerical solution (Du *et al.* 2022). In contrast, the Crank–Nicolson scheme is unconditionally stable for the one-dimensional heat equation and provides second-order accuracy in both time and space (Johnson & Oluwaseun 2020). Prior investigations have primarily focused on theoretical properties such as truncation error (Nagy *et al.* 2022), convergence order (Ali *et al.* 2022), and stability analysis (Dhaouadi *et al.* 2021), with limited attention to systematic parameter optimization. In many numerical simulations, the time-step size is still manually selected using heuristic choices or conservative estimates derived from stability conditions (Sheth *et al.* 2021; Rios *et al.* 2020). Although such approaches usually produce stable numerical solutions, they do not necessarily minimize the approximation error. Different stable time-step values may produce noticeably different numerical results, especially for long-time simulations. Therefore, determining an appropriate time-step size remains an issue for reliable and efficient heat equation simulations.

Several recent studies have explored optimization techniques in heat transfer and diffusion-

related problems. Particle Swarm Optimization (PSO) has been applied in temperature prediction (Liu *et al.* 2024), thermal parameter estimation (Keykhah *et al.* 2020), inverse heat transfer problems (Sun *et al.* 2022), and temperature reconstruction models (Liu *et al.* 2022). These studies demonstrate the usefulness of PSO for parameter estimation problems. However, most existing works focus on physical parameter identification rather than direct optimization of discretization parameters under numerical stability constraints. Adaptive time-stepping and optimization-based parameter selection methods have also received increasing attention in numerical time integration (Smith 2020). Adaptive approaches modify the time-step size according to local error estimates or stability indicators, while optimization-based approaches attempt to improve parameter selection within the admissible stability range. In addition, PSO has gained attention for this type of problem because the objective function is obtained through numerical simulation and does not provide explicit gradient information (Gad 2022). Since the search domain is bounded and low-dimensional, PSO provides a practical derivative-free optimization strategy for identifying suitable parameter values (Chen *et al.* 2024). While these approaches ensure numerical validity, they do not explicitly determine the time-step size that minimizes numerical error. Furthermore, stability constraints are often treated separately from the optimization procedure itself (Shami *et al.* 2022).

To address this issue, this study proposes a stability-constrained optimization approach for time-step selection in finite difference simulations of the one-dimensional heat equation. The time-step selection problem is formulated as a constrained optimization problem within the stability-admissible region. The objective function is defined using the discrete maximum error between the numerical and exact solutions at the final simulation time. Particle Swarm Optimization (PSO) is then employed to determine suitable time-step values automatically. The main contributions of this study are summarized as follows:

- (1) The time-step selection problem is reformulated as a constrained optimization problem under numerical stability conditions.
- (2) A PSO-based search procedure is developed to identify suitable time-step values within the admissible parameter range.
- (3) An automated parameter selection procedure is introduced to reduce dependence on manual trial-and-error tuning.

The proposed formulation combines finite difference analysis with derivative-free optimization for systematic discretization parameter selection. Although the present study focuses on the one-dimensional heat equation, the same formulation can be extended to other parabolic partial differential equation models.

2. Research Methodology

This study investigates the numerical solution of the one-dimensional heat equation using finite difference methods and optimization-based parameter selection. The methodology consists of three main stages. First, the mathematical model of transient heat conduction is formulated. Second, classical finite difference schemes are implemented to approximate the equation. Third, PSO is integrated to automate numerical parameter selection. Numerical experiments are then carried out to evaluate accuracy, convergence behavior, and stability characteristics under controlled discretization settings.

2.1. Mathematical Model

The problem considered in this study is transient heat conduction in a one-dimensional rod of length L . The material is assumed to be homogeneous with constant thermal properties, and heat transfer occurs only through conduction. Under these assumptions, the temperature distribution satisfies the classical one-dimensional heat equation. The heat equation is derived

from the conservation of energy together with Fourier's law of heat conduction (Mevawalla *et al.* 2021; Vinokurov 2014).

Let $u(x, t)$ denote the temperature at position $x \in (0, L)$ and time $t > 0$. The heat equation is given by

$$\frac{\partial u(x, t)}{\partial t} = \alpha \frac{\partial^2 u(x, t)}{\partial x^2}, \quad 0 < x < L, \quad t > 0, \quad (1)$$

where $\alpha > 0$ denotes the thermal diffusivity constant. The Eq. 1 describes the diffusion of heat over time, where temperature differences gradually decrease as the system approaches thermal equilibrium (Kalinay 2025). Next, the initial condition is specified as

$$u(x, 0) = f(x), \quad 0 \leq x \leq L, \quad (2)$$

where $f(x)$ represents the initial temperature distribution along the rod.

Dirichlet boundary conditions are enforced at both ends of the rod, corresponding to fixed temperatures maintained by external thermal reservoirs. These conditions are expressed as

$$u(0, t) = 0, \quad u(L, t) = 0, \quad t \geq 0. \quad (3)$$

Such boundary conditions are commonly adopted in numerical heat transfer studies because they provide a clear physical interpretation and lead to a well-posed initial-boundary value problem with a unique solution (Teixeira *et al.* 2023; Kowalski 2014).

Under the assumption that the initial function $f(x) \in C^2[0, L]$ and the boundary data are sufficiently smooth, the initial-boundary value problem defined by Eqs. 1–3 admits a unique classical solution under standard parabolic regularity theory,

$$u(x, t) \in C^{2,1}((0, L) \times (0, T]) \cap C([0, L] \times [0, T])$$

for any finite $T > 0$. This regularity ensures that the required spatial and temporal derivatives exist and are bounded, thereby justifying the Taylor expansions employed in the truncation error analysis of the finite difference schemes in subsequent sections.

Although analytical solutions to the one-dimensional heat equation can be obtained for certain simple choices of $f(x)$ and boundary conditions using separation of variables, these solutions are limited in scope and often impractical for general discretized simulations (Bağlan & Aslan 2024). Analytical expressions do not readily accommodate flexible numerical parameter selection or automated error minimization. Consequently, numerical approximation techniques are required to compute the temperature field at discrete spatial and temporal locations. The mathematical model presented in this subsection serves as the foundation for the development and assessment of finite difference schemes. It allows the numerical accuracy, stability, and convergence behaviour to be examined under optimized parameter settings in the subsequent sections.

2.2. Analytical Solution for Validation

An analytical solution of the one-dimensional heat equation is used to evaluate the numerical error. Consider the initial condition

$$u(x, 0) = f(x) = \sin(\pi x), \quad 0 \leq x \leq 1, \quad (4)$$

together with homogeneous Dirichlet boundary conditions

$$u(0, t) = 0, \quad u(1, t) = 0, \quad t \geq 0.$$

For the initial condition in Eq. 4, the exact solution is

$$u_{\text{exact}}(x, t) = \sin(\pi x) e^{-\pi^2 \alpha t}. \quad (5)$$

Substituting Eq. 5 into Eq. 1 confirms that the solution satisfies the heat equation.

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2},$$

since

$$\frac{\partial u_{\text{exact}}}{\partial t} = -\pi^2 \alpha \sin(\pi x) e^{-\pi^2 \alpha t}, \quad \frac{\partial^2 u_{\text{exact}}}{\partial x^2} = -\pi^2 \sin(\pi x) e^{-\pi^2 \alpha t}.$$

Hence,

$$\frac{\partial u_{\text{exact}}}{\partial t} = \alpha \frac{\partial^2 u_{\text{exact}}}{\partial x^2}.$$

The solution also satisfies the prescribed boundary conditions since $\sin(0) = \sin(\pi) = 0$, and the initial condition is recovered at $t = 0$.

The exact solution is used as a reference for evaluating the numerical error. For a numerical approximation u_i^n at the final simulation time T , the error is measured using the discrete maximum norm

$$E(\Delta t) = \max_{0 \leq i \leq N} |u_i^n - u_{\text{exact}}(x_i, T)|. \quad (6)$$

This formulation ensures that the numerical schemes are assessed against an exact analytical benchmark rather than a reference numerical approximation, thereby strengthening the mathematical validity of the convergence and optimization analysis presented in subsequent sections.

The discrete maximum norm is used because it measures the largest pointwise difference between the numerical and exact solutions. In heat transfer problems, local errors may remain important even when the overall average error is small. Compared with average-based measures such as the L_2 -norm or root mean square error, the maximum norm is more sensitive to large local deviations. The maximum norm is also commonly used in the stability and convergence analysis of parabolic partial differential equations. In this study, it provides a simple scalar objective function for the PSO procedure, allowing different time-step values to be compared directly.

2.3. Numerical Discretization and Finite Difference Schemes

To numerically approximate the one-dimensional heat equation in Eqs. 1–3, the spatial interval $[0, L]$ is divided into N uniform subintervals with grid spacing $\Delta x = L/N$ and grid points $x_i = i\Delta x$ for $i = 0, 1, \dots, N$. The time domain is discretized with a constant time-step $\Delta t > 0$ and time levels $t^n = n\Delta t$ for $n = 0, 1, 2, \dots$. Let u_i^n denote the numerical approximation of $u(x_i, t^n)$, i.e.,

$$u_i^n \approx u(x_i, t^n).$$

Finite difference methods approximate the derivatives in Eq. 1 by algebraic expressions formed from neighboring grid values. The resulting schemes can be analyzed using Taylor series expansions to determine their truncation errors, accuracy orders, and stability behavior (Liu & Sen 2009).

2.3.1. Taylor expansions and finite-difference operators

For a sufficiently smooth function $u(x, t)$, Taylor expansions about (x_i, t^n) yield

$$u(x_i, t^{n+1}) = u(x_i, t^n) + \Delta t u_t(x_i, t^n) + \frac{\Delta t^2}{2} u_{tt}(x_i, t^n) + \mathcal{O}(\Delta t^3), \quad (7)$$

$$\begin{aligned} u(x_{i\pm 1}, t^n) &= u(x_i, t^n) \pm \Delta x u_x(x_i, t^n) + \frac{\Delta x^2}{2} u_{xx}(x_i, t^n) \\ &\pm \frac{\Delta x^3}{6} u_{xxx}(x_i, t^n) + \frac{\Delta x^4}{24} u_{xxxx}(x_i, t^n) + \mathcal{O}(\Delta x^5) \end{aligned} \quad (8)$$

From Eq. 7, the forward difference approximation to the time derivative is

$$\frac{u(x_i, t^{n+1}) - u(x_i, t^n)}{\Delta t} = u_t(x_i, t^n) + \frac{\Delta t}{2} u_{tt}(x_i, t^n) + \mathcal{O}(\Delta t^2), \quad (9)$$

and from Eq. 8, the central difference approximation to the second spatial derivative is

$$\frac{u(x_{i+1}, t^n) - 2u(x_i, t^n) + u(x_{i-1}, t^n))}{\Delta x^2} = u_{xx}(x_i, t^n) + \frac{\Delta x^2}{12} u_{xxxx}(x_i, t^n) + \mathcal{O}(\Delta x^4). \quad (10)$$

These expansions form the basis for deriving the FTCS and Crank–Nicolson schemes and their truncation errors.

2.3.2. Forward time central space (FTCS) scheme

Applying Eq. 9 and Eq. 10 to the heat equation Eq. 1 at (x_i, t^n) gives

$$\frac{u(x_i, t^{n+1}) - u(x_i, t^n)}{\Delta t} = \alpha \frac{u(x_{i+1}, t^n) - 2u(x_i, t^n) + u(x_{i-1}, t^n))}{\Delta x^2} + \tau_{\text{FTCS}}(x_i, t^n), \quad (11)$$

where τ_{FTCS} denotes the local truncation error. Replacing $u(x_i, t^n)$ by the grid function u_i^n yields the explicit update

$$u_i^{n+1} = u_i^n + r (u_{i+1}^n - 2u_i^n + u_{i-1}^n), \quad i = 1, 2, \dots, N-1, \quad (12)$$

with the Fourier number

$$r = \frac{\alpha \Delta t}{(\Delta x)^2}. \quad (13)$$

The Dirichlet boundary conditions are enforced by setting $u_0^n = 0$ and $u_N^n = 0$ for all n .

Local truncation error and order of accuracy. Substituting Eq. 9 and Eq. 10 into Eq. 11 gives

$$u_t + \frac{\Delta t}{2} u_{tt} + \mathcal{O}(\Delta t^2) = \alpha \left(u_{xx} + \frac{\Delta x^2}{12} u_{xxxx} + \mathcal{O}(\Delta x^4) \right) + \tau_{\text{FTCS}}.$$

Since the governing heat equation satisfies

$$u_t = \alpha u_{xx},$$

the leading-order terms on both sides are identical and therefore cancel exactly. Rearranging the remaining higher-order terms yields the local truncation error

$$\tau_{\text{FTCS}}(x_i, t^n) = \frac{\Delta t}{2} u_{tt}(x_i, t^n) - \alpha \frac{\Delta x^2}{12} u_{xxxx}(x_i, t^n) + \mathcal{O}(\Delta t^2) + \mathcal{O}(\Delta x^4). \quad (14)$$

Hence, the FTCS method is first-order accurate in time and second-order accurate in space:

$$\tau_{\text{FTCS}} = \mathcal{O}(\Delta t) + \mathcal{O}(\Delta x^2).$$

Stability condition. A standard von Neumann stability analysis for Eq. 12 yields the conditional stability requirement (Dhaouadi *et al.* 2021; Wen-ping 2000)

$$0 \leq r \leq \frac{1}{2}, \quad (15)$$

which imposes the time-step restriction $\Delta t \leq (\Delta x)^2/(2\alpha)$.

2.3.3. Crank–Nicolson scheme

The Crank–Nicolson method is obtained by averaging the spatial discretization at time levels t^n and t^{n+1} . Specifically, we approximate u_t by a centered difference in time and u_{xx} by the average of central differences:

$$\begin{aligned} \frac{u(x_i, t^{n+1}) - u(x_i, t^n)}{\Delta t} &= \frac{\alpha}{2} \left[\frac{u(x_{i+1}, t^{n+1}) - 2u(x_i, t^{n+1}) + u(x_{i-1}, t^{n+1}))}{\Delta x^2} \right. \\ &\quad \left. + \frac{u(x_{i+1}, t^n) - 2u(x_i, t^n) + u(x_{i-1}, t^n))}{\Delta x^2} \right] \\ &\quad + \tau_{\text{CN}}(x_i, t^n). \end{aligned} \quad (16)$$

Replacing the exact values with u_i^n gives the implicit tridiagonal system

$$-ru_{i-1}^{n+1} + (1+2r)u_i^{n+1} - ru_{i+1}^{n+1} = ru_{i-1}^n + (1-2r)u_i^n + ru_{i+1}^n, \quad i = 1, 2, \dots, N-1, \quad (17)$$

where r is defined in Eq. 13. The boundary conditions are enforced by $u_0^n = 0$ and $u_N^n = 0$.

Local truncation error and order of accuracy. To obtain the truncation error, note that the left-hand side of Eq. 16 is a first-order forward difference in time and thus has expansion Eq. 9. However, the right-hand side uses the average of spatial second derivatives at t^n and t^{n+1} . Using Eq. 10 at both time levels and Taylor expanding $u_{xx}(x_i, t^{n+1})$ about t^n ,

$$u_{xx}(x_i, t^{n+1}) = u_{xx}(x_i, t^n) + \Delta t u_{xxt}(x_i, t^n) + \frac{\Delta t^2}{2} u_{xxtt}(x_i, t^n) + \mathcal{O}(\Delta t^3),$$

the Crank–Nicolson scheme introduces symmetry in time by averaging the spatial discretization at two consecutive time levels. This averaging eliminates the first-order temporal truncation term that appears in explicit forward differencing and produces a midpoint approximation in time. Consequently, the averaged spatial term approximates u_{xx} at the temporal midpoint with

second-order accuracy, leading to

$$\tau_{\text{CN}}(x_i, t^n) = \mathcal{O}(\Delta t^2) + \mathcal{O}(\Delta x^2). \quad (18)$$

Therefore, the Crank–Nicolson scheme is second-order accurate in time and second-order accurate in space:

$$\tau_{\text{CN}} = \mathcal{O}(\Delta t^2) + \mathcal{O}(\Delta x^2).$$

Stability. For the one-dimensional heat equation, Crank–Nicolson is unconditionally stable in the von Neumann sense, meaning that stability does not impose a restriction on Δt for fixed Δx (Johnson & Oluwaseun 2020; Liu & Hao 2022). This allows larger time-step sizes compared with the FTCS method, although accuracy considerations still require Δt to be chosen appropriately.

2.3.4. Comparative numerical framework

In this study, the time-step size Δt is selected as the main discretization parameter. For the FTCS scheme, the time step must satisfy Eq. 15. In contrast, the Crank–Nicolson scheme can be evaluated over a wider range of time-step values because it is unconditionally stable. Both schemes are initialized using the same $f(x)$ and advanced to the same final time T , with numerical solutions stored for subsequent error, convergence, and stability analyses. This consistent setup also facilitates the integration of optimization techniques for systematic parameter selection.

2.3.5. Consistency, stability and convergence

The FTCS and Crank–Nicolson schemes derived above are consistent with the heat equation, as evidenced by their respective local truncation errors

$$\tau_{\text{FTCS}} = \mathcal{O}(\Delta t) + \mathcal{O}(\Delta x^2), \quad \tau_{\text{CN}} = \mathcal{O}(\Delta t^2) + \mathcal{O}(\Delta x^2).$$

For the FTCS scheme, stability is ensured under the restriction

$$0 \leq r = \frac{\alpha \Delta t}{(\Delta x)^2} \leq \frac{1}{2},$$

while the Crank–Nicolson scheme is unconditionally stable for the one-dimensional heat equation.

Under the smoothness assumptions stated in Section 2.1 and the corresponding stability conditions, both schemes are convergent. In particular, the global error at the final time T satisfies

$$\|u(\cdot, T) - u^{n_T}\|_\infty = \begin{cases} \mathcal{O}(\Delta t + \Delta x^2), & \text{FTCS,} \\ \mathcal{O}(\Delta t^2 + \Delta x^2), & \text{Crank–Nicolson.} \end{cases}$$

This follows from the classical equivalence principle for linear parabolic problems. The dominant temporal error term therefore determines the sensitivity of each scheme to the time-step size. Consequently, the time discretization parameter plays a central role in controlling overall numerical accuracy, thereby motivating its treatment as an optimization variable in the subsequent section.

2.4. Particle Swarm Optimization for Parameter Selection

The time-step size Δt plays a central role in determining numerical accuracy, stability, and computational cost in finite difference simulations (Mathias 2024). From a numerical perspective, Δt affects both the approximation error and the computational cost. Smaller values of Δt generally improve numerical accuracy but require more iterations to reach the final simulation time. On the other hand, excessively large time-step values may produce unstable numerical solutions. Stability constraints impose an upper bound on the allowable Δt to prevent divergence of the numerical solution. For the FTCS scheme, the time-step value must satisfy the stability condition, whereas the Crank–Nicolson scheme allows a wider range of values due to unconditional stability. However, satisfying the stability condition alone does not guarantee minimum numerical error. Different stable values of Δt may still produce noticeably different approximation errors and computational costs. Therefore, the time-step selection problem is formulated as a constrained optimization problem instead of relying solely on manual parameter selection.

To automate the parameter selection process, PSO is used as a derivative-free metaheuristic method. Particle Swarm Optimization (PSO) systematically explores the valid parameter space and identifies near-optimal solutions based on the defined objective function. The candidate solutions are updated iteratively through cooperative search behaviour (Gad 2022; Kennedy & Eberhart 1995). Since the optimization problem considered here is bounded and low-dimensional, PSO provides a practical approach for exploring the admissible parameter range. In the present formulation, each particle represents a candidate time-step value Δt . The search interval is restricted according to the stability condition of the numerical scheme. For FTCS, the stability condition

$$r = \frac{\alpha \Delta t}{(\Delta x)^2} \leq \frac{1}{2}$$

must be satisfied. On the other hand, the Crank–Nicolson scheme does not require the same conditional stability restriction.

Let $u_{\text{num}}(x_i, T; \Delta t)$ denote the numerical solution at the final time T obtained using a given time-step value, and let $u_{\text{exact}}(x_i, T)$ denote the corresponding exact solution. The optimization objective is defined using the discrete maximum norm so that the selected time-step value minimizes the largest pointwise numerical error. It is formulated as

$$J(\Delta t) = \max_{0 \leq i \leq N} |u_{\text{num}}(x_i, T; \Delta t) - u_{\text{exact}}(x_i, T)|. \quad (19)$$

Although the objective function is defined using the discrete maximum-norm error, it captures the interaction between truncation error and computational cost.

The time-step selection problem is therefore expressed as

$$\Delta t^* = \arg \min_{\Delta t \in \mathcal{D}} J(\Delta t),$$

where $\mathcal{D}$ denotes the valid set of time-step values defined by the stability constraints of the underlying numerical scheme. For the FTCS method, this domain is restricted by the condition

$$\Delta t \leq \frac{(\Delta x)^2}{2\alpha},$$

while for the Crank–Nicolson scheme, the stability-constrained domain is determined by practical accuracy considerations rather than stability restrictions. The domain $\mathcal{D}$ ensures that all candidate solutions generated during the optimization process remain numerically stable and physically valid, thereby embedding stability constraints directly into the optimization framework. Since $J(\Delta t)$ is evaluated via discrete numerical simulations, explicit gradient informa-

tion is unavailable, which motivates the use of a derivative-free optimization strategy.

2.4.1. Existence and structure of the optimal time-step

To provide theoretical support for the optimization framework, we analyze the existence and asymptotic behavior of the optimal time-step. Let $J(\Delta t)$ defined in Eq. 19 denote the discrete maximum-norm error functional over the stability-constrained domain

$$\mathcal{D} = [\Delta t_{\min}, \Delta t_{\max}],$$

where $\Delta t_{\max}$ satisfies the stability restriction for the FTCS scheme. For fixed spatial discretization and finite final time T , the discrete numerical solution depends continuously on Δt . Consequently, the functional $J(\Delta t)$ is continuous on the compact interval $\mathcal{D}$. By the extreme value theorem, there exists at least one minimizer

$$\Delta t^* = \arg \min_{\Delta t \in \mathcal{D}} J(\Delta t).$$

Furthermore, from the global error estimates established in Section 2.3, the leading-order temporal contributions satisfy

$$J(\Delta t) \approx \begin{cases} C_1 \Delta t + C_2 \Delta x^2, & \text{FTCS,} \\ C_3 \Delta t^2 + C_4 \Delta x^2, & \text{Crank-Nicolson,} \end{cases}$$

for positive constants C_1, C_2, C_3 , and C_4 independent of Δt and Δx . This asymptotic structure indicates that the optimal time-step is expected to exhibit scaling behaviour of the form

$$\Delta t^* = O(\Delta x^2),$$

particularly for the explicit scheme, where temporal and spatial error components balance. The optimization procedure therefore provides a numerical mechanism for approximating this theoretically predicted optimal scaling without requiring explicit knowledge of the associated constants.

2.4.2. PSO algorithm

To approximate the minimizer Δt^* , PSO is employed as a derivative-free search strategy over the stability-constrained domain $\mathcal{D}$. Each particle in the swarm represents a candidate time-step value $\Delta t_p^{(k)}$ at iteration k , together with an associated velocity $v_p^{(k)}$. The particle velocities and positions are updated according to

$$\begin{aligned} v_p^{(k+1)} &= \omega v_p^{(k)} + c_1 r_1 (pbest_p - \Delta t_p^{(k)}) + c_2 r_2 (gbest - \Delta t_p^{(k)}), \\ \Delta t_p^{(k+1)} &= \Delta t_p^{(k)} + v_p^{(k+1)}, \end{aligned}$$

where ω denotes the inertia weight, c_1 and c_2 are acceleration coefficients, and $r_1, r_2 \sim \mathcal{U}(0, 1)$ are independent random variables. The quantities $pbest_p$ and $gbest$ denote the best position obtained by particle p and the best position found by the swarm, respectively.

After each update, the time-step value is checked to ensure that $\Delta t_p^{(k+1)} \in \mathcal{D}$. For the FTCS scheme, the stability condition

$$\frac{\alpha \Delta t_p^{(k+1)}}{(\Delta x)^2} \leq \frac{1}{2}$$

must be satisfied. The objective function $J(\Delta t_p^{(k+1)})$ is then evaluated, followed by updates of the personal and global best positions. The iterations continue until the maximum number of iterations is reached or the improvement in the objective value becomes sufficiently small.

2.4.3. PSO parameter specification

Since the optimization problem involves only a single variable, namely the time-step size Δt , a moderate swarm size is sufficient for the present computation. The swarm size M controls the diversity of candidate solutions explored during the search. A moderate swarm size is preferred to ensure sufficient exploration of the stability-constrained domain. The inertia weight ω regulates the influence of previous particle velocities and determines the balance between global exploration and local exploitation. Larger values of ω encourage broader search behavior, while smaller values promote faster local convergence near the optimum. The acceleration coefficients c_1 and c_2 control the relative attraction toward the personal best position and the global best position, respectively. In this study, the PSO uses a swarm size of $M = 30$ particles, inertia weight $\omega = 0.72984$, and acceleration coefficients $c_1 = c_2 = 1.496172$, following the standard constriction-factor parameter setting reported by Clerc and Kennedy (2002). This configuration is particularly suitable for the bounded and smooth optimization landscape associated with finite difference time-step selection.

The particle positions are initialized uniformly within the admissible interval $\mathcal{D}$, together with randomly generated initial velocities. During each iteration, the updated time-step values are checked against the stability condition for the FTCS scheme. The objective function is then evaluated, and the particle positions are updated accordingly. The iterations continue until either the maximum number of iterations $I_{\max}$ is reached or the improvement in the global best objective value becomes sufficiently small (less than ε).

2.5. Numerical Experiment Design

Numerical experiments are performed to evaluate the accuracy, convergence, and stability behaviour of the finite difference schemes. The one-dimensional spatial domain is discretized using a uniform grid with a fixed number of spatial nodes. The spatial discretization is kept unchanged throughout the simulations so that the effect of the time-step size can be examined directly. The same initial condition and Dirichlet boundary conditions are used in all simulations. Each computation is carried out up to the same final time T for comparison of the numerical solutions. The numerical accuracy is assessed by comparing the computed solutions with the analytical solution given in Eq. 5. The numerical error is measured using the maximum absolute difference at the final simulation time, as defined in Eq. 19. This experimental protocol provides a consistent and reproducible framework for evaluating numerical performance prior to optimization.

2.5.1. Computational implementation

All numerical simulations and optimization procedures are implemented in MATLAB using a modular programming structure. Separate function files are developed for the FTCS and Crank–Nicolson schemes, each accepting identical input parameters, including initial condition, thermal diffusivity α , spatial step size Δx , time-step size Δt , and final simulation time T . A closed-form analytical solution, given in Eq. 5, is used as the reference benchmark for numerical validation. For each simulation, the exact solution is evaluated at the spatial grid points at the final simulation time. The numerical error is computed as the maximum absolute difference between the numerical approximation and the analytical solution at the final time. This error measure is used as the objective function in the time-step sensitivity analysis and PSO optimization procedure. The analytical solution provides a direct reference for computing the numerical error throughout the study.

Particle Swarm Optimization (PSO) is implemented in the MATLAB environment and coupled with the finite difference solvers. Each particle represents a candidate time-step value Δt . For every candidate value, the numerical solution and corresponding error are computed using the selected finite difference scheme. The personal and global best positions are updated iteratively during the optimization process. Additional scripts are used to generate error-versus-time-step plots and convergence curves for further analysis. The overall computational procedure is summarized in Algorithm 1.

Algorithm 1 PSO-Integrated Finite Difference Solver for the 1D Heat Equation

Input: Rod length L ; final time T ; thermal diffusivity α ; number of spatial intervals N ; initial condition $u(x, 0) = f(x)$; Dirichlet boundary conditions $u(0, t) = u(L, t) = 0$.

PSO parameters: Swarm size P ; maximum iterations $I_{\max}$; inertia weight ω ; acceleration constants c_1 and c_2 .

Search bounds: $\Delta t \in [\Delta t_{\min}, \Delta t_{\max}]$. For FTCS, the stability condition must satisfy

$$r = \frac{\alpha \Delta t}{\Delta x^2} \leq \frac{1}{2}.$$

Output: Optimised time step Δt^* ; optimised solution $u^*(x, t)$; minimum error J^* .

Step A: Discretisation and Reference Solution

1. Set

$$\Delta x = \frac{L}{N}, \quad x_i = i\Delta x, \quad i = 0, 1, \dots, N.$$

2. Construct the initial vector

$$u^0 = [f(x_0), f(x_1), \dots, f(x_N)]^T.$$

3. Enforce the boundary values

$$u_0^n = 0, \quad u_N^n = 0$$

for all n .

4. Evaluate the exact solution $u_{\text{exact}}(x, T)$ using Eq. 5.

Step B: Objective Function

For a candidate time step Δt , define

$$J(\Delta t) = \|u(T; \Delta t) - u_{\text{ref}}(T)\|_{\infty} = \max_{0 \leq i \leq N} |u_i(T; \Delta t) - u_{\text{ref},i}(T)|.$$

Here, $u(T; \Delta t)$ is computed using either FTCS or Crank–Nicolson.

Step C: PSO Optimisation Loop

For each scheme $S \in \{\text{FTCS}, \text{CN}\}$, determine

$$\Delta t_S^* = \arg \min_{\Delta t \in [\Delta t_{\min}, \Delta t_{\max}]} J_S(\Delta t).$$

5. Initialise particles

$$\Delta t_p^{(0)} \sim \mathcal{U}[\Delta t_{\min}, \Delta t_{\max}], \quad p = 1, \dots, P.$$

6. Initialise velocities $v_p^{(0)}$.
7. Set personal bests

$$pbest_p = \Delta t_p^{(0)}.$$

8. Evaluate

$$J_p^{(0)} = J_S \left(\Delta t_p^{(0)} \right).$$

9. Set the global best

$$gbest = \arg \min_p J_p^{(0)}.$$

10. For $k = 0, 1, \dots, I_{\max} - 1$:

- (a) For each particle p :
Update the velocity:

$$v_p^{(k+1)} = \omega v_p^{(k)} + c_1 r_1 \left(pbest_p - \Delta t_p^{(k)} \right) + c_2 r_2 \left(gbest - \Delta t_p^{(k)} \right).$$

Update the position:

$$\Delta t_p^{(k+1)} = \Delta t_p^{(k)} + v_p^{(k+1)}.$$

Apply the search bounds:

$$\Delta t_p^{(k+1)} \leftarrow \min \left\{ \Delta t_{\max}, \max \left[\Delta t_{\min}, \Delta t_p^{(k+1)} \right] \right\}.$$

For FTCS, enforce

$$r = \frac{\alpha \Delta t_p^{(k+1)}}{\Delta x^2} \leq \frac{1}{2},$$

which implies

$$\Delta t_p^{(k+1)} \leq \frac{\Delta x^2}{2\alpha}.$$

Evaluate

$$J_p^{(k+1)} = J_S \left(\Delta t_p^{(k+1)} \right).$$

If

$$J_p^{(k+1)} < J_S(pbest_p),$$

then update

$$pbest_p \leftarrow \Delta t_p^{(k+1)}.$$

(b) Update the global best:

$$gbest \leftarrow \arg \min_p J_p^{(k+1)}.$$

(c) Stop if the convergence criterion is satisfied or if $k = I_{\max} - 1$.

11. Return

$$\Delta t_S^* = gbest, \quad J_S^* = J_S(\Delta t_S^*).$$

Step D: Final Optimised Simulation

12. Using Δt_S^* , compute the final numerical solution

$$u_S^*(T).$$

13. Report Δt_S^* , J_S^* , and the corresponding temperature profile.

3. Results and Discussion

The stability-admissible optimization framework described in Section 2 is now evaluated through controlled computational experiments. This section presents numerical results obtained from the finite difference simulations and analyzes their implications in terms of accuracy, stability, and optimization-driven parameter selection. The numerical results are first examined through the temperature distributions produced by the FTCS and Crank–Nicolson schemes before proceeding to the error and convergence analysis.

3.1. Temperature Distribution Profiles

Figure 1(a) and Figure 1(b) show the temperature distributions at the final simulation time obtained using the FTCS and Crank–Nicolson schemes, respectively. Both solutions produce smooth symmetric profiles with the highest temperature occurring near the center of the rod and zero temperature at the boundaries. This behaviour agrees with the expected diffusion pattern for the one-dimensional heat equation under Dirichlet boundary conditions.

The two numerical profiles are visually similar, indicating that both schemes produce comparable solutions for sufficiently small time-step values. No noticeable difference is observed at this stage, suggesting that both numerical methods are able to capture the overall heat diffusion behaviour of the system. These results provide qualitative validation before proceeding to quantitative error analysis in the following section. The validation step ensures that subsequent optimization results are evaluated on physically consistent numerical solutions to isolate the effect of time-step selection.

3.2. Error Comparison

Table 1 compares the peak temperature values and maximum absolute errors obtained using the FTCS and Crank–Nicolson schemes for different time-step sizes. The reference peak temperature is computed from the exact solution in Eq. 5 at the final simulation time.

For all tested time-step values, the Crank–Nicolson scheme produces very small numerical errors that remain close to machine precision. The FTCS scheme, however, shows increasing error as the time-step size becomes larger, even when the stability condition is satisfied. Although both schemes produce similar peak temperature values, the FTCS results are noticeably

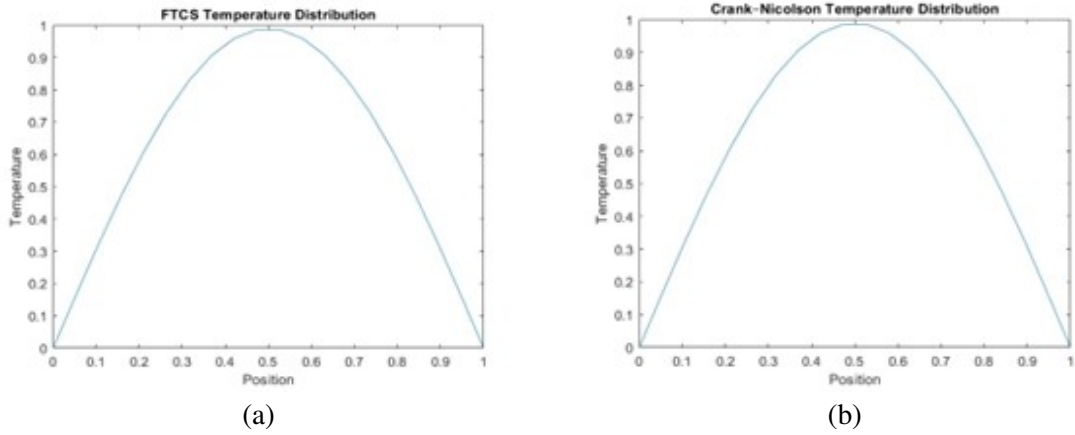


Figure 1: Temperature distributions at the final simulation time obtained using (a) the FTCS scheme and (b) the Crank–Nicolson scheme

Table 1: Peak temperature values and maximum absolute errors for the FTCS and Crank–Nicolson schemes under different time-step sizes

Time-step Δt	FTCS peak	FTCS error	CN peak	CN error
1.0×10^{-5}	0.98682	4.7846×10^{-9}	0.98682	$< 10^{-15}$
5.0×10^{-4}	0.98682	2.3923×10^{-7}	0.98682	2.1964×10^{-12}
1.0×10^{-3}	0.98682	4.7847×10^{-7}	0.98682	8.0668×10^{-12}
2.0×10^{-3}	0.98682	9.5701×10^{-7}	0.98682	3.1642×10^{-11}

more sensitive to the choice of Δt . This suggests that the dominant source of error in FTCS arises from temporal discretization.

Figure 2 shows the relationship between the maximum absolute error and the time-step size for both numerical schemes. For FTCS, the error increases approximately linearly with Δt , which is consistent with the first-order temporal truncation error $\mathcal{O}(\Delta t)$ derived in Section 2.3. Similar behaviour has been reported for explicit finite difference methods in classical numerical analysis studies (LeVeque 2007). These results show that stable time-step values may still produce noticeably different numerical errors. Stability ensures boundedness of the solution but does not guarantee optimal accuracy. This shows the need for parameter selection driven by optimization within the stability-constrained domain.

The Crank–Nicolson scheme maintains a much smaller error over the tested range of time-step values. This is consistent with its second-order temporal accuracy $\mathcal{O}(\Delta t^2)$ and unconditional stability for the one-dimensional heat equation. The error variation remains relatively small even when larger values of Δt are used, indicating lower sensitivity to time discretization compared with FTCS. The nearly flat error profile observed for Crank–Nicolson demonstrates strong robustness against time discretization changes and confirms the practical advantage of implicit finite difference schemes for reliable simulations.

3.3. Experimental Order of Convergence

To verify the theoretical truncation error analysis presented in Section 2.3, the experimental order of convergence (EOC) is computed with respect to time discretization. Let $E(\Delta t)$ denote the maximum absolute error at the final simulation time corresponding to a given time-step size Δt . For two successive time-step sizes Δt_1 and Δt_2 , the observed convergence rate p is

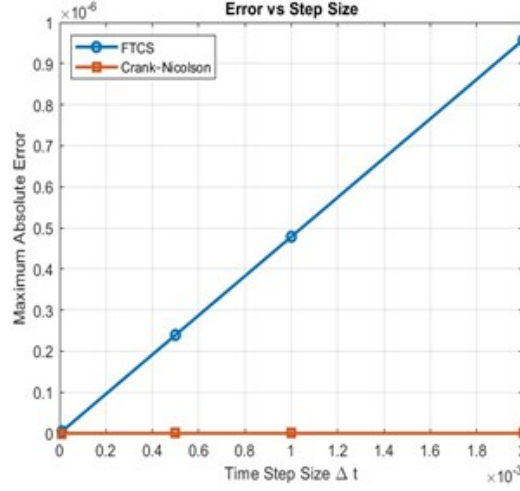


Figure 2: Maximum absolute error as a function of time-step size Δt for the FTCS and Crank–Nicolson schemes

estimated using

$$p = \frac{\log(E(\Delta t_1)/E(\Delta t_2))}{\log(\Delta t_1/\Delta t_2)}. \quad (20)$$

The spatial discretization is kept fixed while the time-step is successively refined. Table 2 reports the numerical errors and the corresponding observed convergence orders for both the FTCS and Crank–Nicolson schemes.

Table 2: Experimental convergence order for FTCS and Crank–Nicolson schemes under time-step refinement.

Δt	FTCS Error	FTCS Order	CN Error	CN Order
2.0×10^{-3}	9.57×10^{-7}	–	3.16×10^{-11}	–
1.0×10^{-3}	4.78×10^{-7}	1.00	8.07×10^{-12}	1.97
5.0×10^{-4}	2.39×10^{-7}	1.00	2.02×10^{-12}	2.00
2.5×10^{-4}	1.20×10^{-7}	1.00	5.05×10^{-13}	2.00

For the FTCS scheme, the observed convergence rates are consistently close to one, confirming first-order temporal accuracy in agreement with the local truncation error analysis,

$$\tau_{\text{FTCS}} = \mathcal{O}(\Delta t) + \mathcal{O}(\Delta x^2).$$

Such convergence behaviour is well documented in the numerical analysis literature for parabolic partial differential equations, where the observed order of convergence closely follows the theoretical truncation error structure (LeVeque 2007). These results validate the theoretical prediction that the dominant temporal error term scales linearly with the time-step size. In practical terms, halving the time-step approximately halves the numerical error, implying that achieving higher accuracy requires substantially smaller time-steps and consequently increased computational cost due to the larger number of iterations required.

In contrast, the Crank–Nicolson scheme exhibits convergence rates close to two, verifying second-order temporal accuracy consistent with the truncation error estimate

$$\tau_{\text{CN}} = \mathcal{O}(\Delta t^2) + \mathcal{O}(\Delta x^2).$$

The reduction in error under successive time-step refinement reflects the second-order temporal accuracy of the Crank–Nicolson scheme. In general, halving the time-step size reduces the temporal error by approximately a factor of four. As a result, relatively larger time-step values can still produce small numerical errors compared with the FTCS scheme. The experimentally observed convergence rates are also consistent with the theoretical convergence orders derived earlier. This agreement indicates that the numerical implementation follows the expected error behaviour for both finite difference schemes.

3.4. PSO Convergence Behavior

Figure 3 shows the convergence history of the PSO algorithm for both numerical schemes. In both cases, the objective value decreases rapidly during the early iterations before approaching a stable value. Only a small number of iterations is required before the improvement becomes negligible. The observed convergence behaviour suggests that the time-step optimization problem is relatively smooth and low-dimensional. Similar convergence patterns for PSO have also been reported in previous numerical optimization studies (Chauhan *et al.* 2025). The results indicate that PSO is able to determine suitable time-step values efficiently for the present problem.

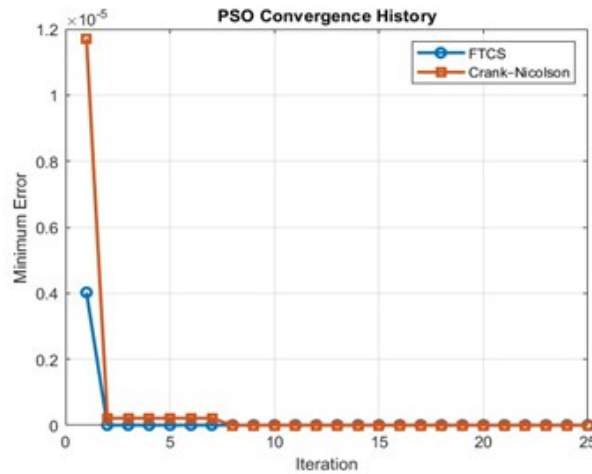


Figure 3: PSO convergence history for the FTCS and Crank–Nicolson schemes

For the FTCS scheme, the optimization process is restricted by the stability condition $r \leq \frac{1}{2}$, which limits the allowable range of time-step values. Within this restricted interval, PSO searches for time-step values that produce smaller numerical error while satisfying the stability requirement. This demonstrates the effectiveness of PSO in automating parameter selection for conditionally stable schemes. On the other hand, Crank–Nicolson scheme allows a wider range of time-step values because it is unconditionally stable. As observed in Figure 3, the convergence process becomes slightly faster for this case since the admissible parameter range is less restricted.

Compared with manual trial-and-error parameter selection, PSO provides an automatic procedure for determining suitable time-step values. Although the optimization process requires repeated objective evaluations, the additional computational cost remains moderate because the optimization problem involves only a single parameter. Each objective evaluation consists of a standard finite difference simulation, which is relatively inexpensive for the present one-dimensional problem. Once the time-step value is selected, the final numerical simulation is performed without further optimization iterations. The results indicate that PSO can be used effectively for automatic time-step selection in finite difference simulations. Compared with

PSO, manual selection of the time-step size often requires repeated simulations using different values of Δt before a suitable parameter can be identified. This may increase the overall computational time required to obtain accurate numerical results.

3.5. Numerical Implications

The numerical results show that the choice of time-step size has a noticeable effect on the accuracy of the finite difference solutions. Although the Crank–Nicolson scheme is unconditionally stable and produces smaller numerical error than FTCS, different values of Δt still lead to different error levels and computational costs. In many numerical simulations, the time-step value is selected manually using fixed small values or estimates based on the CFL condition. While these choices usually produce stable numerical solutions, they do not necessarily give the smallest approximation error.

Table 3 compares the proposed PSO-based time-step selection with several conventional parameter choices using the Crank–Nicolson scheme. The comparison includes a fixed small time-step, a CFL-based selection, and the optimized value obtained using PSO.

Table 3: Comparison of time-step selection methods using the Crank–Nicolson scheme

Method	Selected Δt	Error	CPU Time (s)
Small fixed Δt	2.5×10^{-4}	5.0546×10^{-13}	56
CFL-based heuristic Δt	2.0×10^{-3}	3.1601×10^{-11}	15
Proposed PSO-based method	1.5×10^{-4}	1.5428×10^{-15}	319

The comparison shows that smaller time-step values generally produce lower numerical error but require longer computational time due to the increased number of iterations. This suggests that different stable values of Δt may still lead to significantly different numerical results, even for the Crank–Nicolson scheme. The CFL-based selection gives the shortest computational time, although the numerical error is noticeably larger. Among the tested approaches, the PSO-selected time-step produces the smallest numerical error. The results indicate that optimization-based parameter selection can provide smaller numerical error than fixed or CFL-based choices. This supports the observation that stability conditions alone are insufficient for selecting time-step values that produce accurate numerical solutions.

4. Conclusion

This study investigated time-step selection for finite difference approximations of the one-dimensional heat equation using a stability-constrained optimization approach. The time-step size was treated as an optimization variable, while the numerical error was measured using the discrete maximum norm under the corresponding stability conditions. This formulation allows systematic identification of near-optimal time-step values within the stability-admissible domain. The numerical results showed that different stable values of Δt may still produce noticeably different numerical errors. For the FTCS scheme, the error increased as the time-step size became larger, even within the admissible stability range. In contrast, the Crank–Nicolson scheme maintained smaller numerical error over a wider range of time-step values due to its second-order temporal accuracy and unconditional stability.

Particle Swarm Optimization (PSO) was used to determine suitable time-step values automatically. Compared with fixed and CFL-based parameter choices, the PSO-selected values produced smaller numerical error in the tested simulations. Although the optimization process requires additional objective evaluations, this cost occurs only during parameter selection. The results suggest that stability conditions alone are insufficient for selecting time-step values that

produce accurate numerical solutions. The proposed optimization approach can also be extended to other finite difference models and more general time-dependent partial differential equations.

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