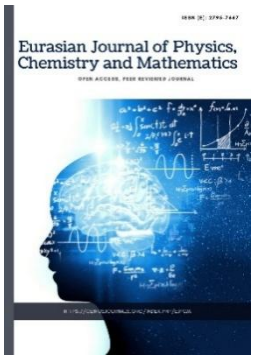

Comparison Of Runge–Kutta, Multistep, And Crank–Nicolson Schemes For Time Integration In The Numerical Solution Of The Heat Equation

Imomova Shafoat Mahmudovna — Assistant Professor, Bukhara State University, Uzbekistan

Hamidova Anora Dovud qizi — Master Of Specialty in Applied Mathematics, Bukhara State University, Uzbekistan

Jo'rayeva Lobar Umid qizi — Master Of Specialty in Applied Mathematics, Bukhara State University, Uzbekistan

ABSTRACT

In this paper, three time-integration approaches for the numerical solution of the one-dimensional heat conduction equation are compared, namely one-step Runge–Kutta methods, Adams-type multistep methods, and the Crank–Nicolson scheme. As a model problem we consider the classical heat equation with Dirichlet boundary conditions, discretized in space by second-order central finite differences. The resulting system of linear ODEs is integrated in time using the fourth-order Runge–Kutta method, the three-step Adams–Bashforth–Moulton predictor–corrector pair, and the Crank–Nicolson scheme, which is equivalent to the trapezoidal rule. We analyze the local and global orders of accuracy, stability properties, and computational efficiency of these methods. For a test problem with known analytical solution, the errors are measured in the L_2 and L_∞ norms, and the influence of the time step and spatial step is illustrated using tables and plots. The results show that for sufficiently small-time steps, the Runge–Kutta method provides the highest accuracy, while multistep methods offer a compromise between accuracy and efficiency. The Crank–Nicolson scheme, due to its unconditional stability, yields stable solutions even for relatively large time steps, at the cost of solving a linear system at each step. The findings provide practical guidelines for choosing time-integration methods for the heat equation and similar parabolic partial differential equations.

Keywords: heat equation, Runge–Kutta methods, multistep methods, Adams–Bashforth, Adams–Moulton, Crank–Nicolson scheme, stability, global error, finite differences

1. Introduction

The heat conduction equation is one of the most widely used models among parabolic partial differential equations (PDEs) and is applied in the simulation of heat transfer in solid bodies, building walls, electronic boards, and many other systems. Exact analytical solutions are available only for relatively simple geometries, homogeneous coefficients, and simple initial–boundary conditions. Therefore, the majority of practical problems are solved by numerical methods.

For parabolic equations, a standard numerical approach is to discretize the spatial variables using finite differences, finite elements, or spectral methods and then to integrate the resulting system of ordinary differential equations (ODEs) in time. For time integration, two main classes of methods are commonly used: (i) one-step Runge–Kutta

methods and (ii) linear multistep methods such as Adams–Bashforth and Adams–Moulton schemes.

In addition, the Crank–Nicolson scheme, specifically designed for diffusion-type problems, is widely used. It is a second-order accurate implicit method in both space and time, equivalent to applying the trapezoidal rule in time to the semi-discrete system. For the heat equation, it is well known to be unconditionally stable.

The objective of this paper is to compare, both theoretically and numerically, the fourth-order Runge–Kutta method, Adams-type predictor–corrector multistep methods, and the Crank–Nicolson scheme as time integrators for the one-dimensional heat equation. We aim to highlight their advantages and limitations and to provide practical recommendations on when each method is preferable.

2. Model Equation and Spatial Discretization

Heat equation

We consider the one-dimensional heat equation in the interval $(0, L)$:

$$u_t(x,t) = \alpha u_{xx}(x,t), \qquad 0 < \mathrm{x} < \mathrm{L}, \qquad 0 < \mathrm{t} \leq \mathrm{T}$$

Where $\alpha > 0$ is the thermal diffusivity ,and $u(x,t)$ is the temperature.We prescribe homogeneous Dirichlet boundary conditions:

$$u(0,t) = 0, \; u(L,t) = 0, \qquad 0 < t \leq T,$$

and an initial condition

$$u(x,0) = u_0(x), \qquad 0 \leq x \leq L.$$

For the numerical tests we choose a problem with a known analytical solution by taking

$$u_0(x) = \sin(\pi x/L), \quad L = 1.$$

In this case the analytical solution is

$$u(x,t) = e^{-\alpha\pi^2 t} \sin(\pi x),$$

which will be used as a reference to assess the accuracy of the numerical methods .

Spatial discretization

We discretize the interval [0,1] using a uniform grid:

$$x_j = jh, \quad j = 0,1,\dots,N, \qquad h = \frac{1}{N}.$$

A second-order central difference approximation for the second derivative gives

$$u_{xx}(x_j,t) \approx \frac{u_{j+1}(t) - 2u_j(t) + u_{j-1}(t)}{h^2}$$

where $u_j(t) \approx u(x_j, t)$. For interior nodes $j = 1, \dots, N-1$:

$$\frac{du_j}{dt} = \alpha \frac{u_{j+1} - 2u_j + u_{j-1}}{h^2}.$$

The boundary conditions are imposed as

$$u_0\,(t) = 0, \qquad u_N(t) = 0.$$

In vector form we write

$$\frac{\mathrm{dU}}{\mathrm{dt}} = \mathrm{AU}, \quad \mathrm{U}(0) = \mathrm{U}_{0,}$$

where $U(t) = [u_1(t), \dots, u_{N-1}(t)]^T$, and A is the tri-diagonal matrix

$$A = \frac{\alpha}{h^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}$$

Thus, the PDE problem is reduced to a linear system of ODEs, and the main task becomes the choice and comparison of time-stepping methods for this system.

3. Runge–Kutta and multistep methods for time integration

Runge–Kutta methods

Runge–Kutta methods are one-step schemes for the ODE

$$y' = f(t, y),$$

with the general form

$$y_{n+1} = y_n + \Delta t \sum_{i=1}^{s} b_i\, k_i,$$

$$k_i = f\left(t_n + c_i \Delta t, y_n + \Delta t \sum_{j=1}^{s} a_{ij} k_j\right), \quad i = 1, \dots, s.$$

The most widely used scheme is the classical fourth-order Runge–Kutta (RK4) method:

$$k_1 = f(t_n, y_n),$$
$$k_2 = f\left(t_n + \frac{\Delta t}{2}, y_n + \frac{\Delta t}{2} k_1\right),$$
$$k_3 = f\left(t_n + \frac{\Delta t}{2}, y_n + \frac{\Delta t}{2} k_2\right),$$
$$k_4 = f(t_n + \Delta t, y_n + \Delta t k_3),$$

$$y_{n+1} = y_n + \frac{\Delta t}{6}(k_1 + 2k_2 + 2k_3 + k_4).$$

This method has local truncation error of order $O(\Delta t^5)$ and global error of order $O(\Delta t^4)$.For the semi-discrete heat equation, the right-hand side is linear,$f(t, U) = AU$,therefore RK4 can be implemented efficiently, requiring only matrix-vector multiplications.

However, the heat equation is parabolic, and the eigenvalues of A satisfy $p(A) \sim O(h^{-2})$. As a result, explicit methods such as RK4 are subjects to a stability constraint of the form

$$\Delta t \le C h^2,$$

with some constant CCC, so that when the spatial grid is refined, the time step must be significantly reduced.

Adams-type multistep methods

Linear multistep methods compute the next value using several previous steps.The general s-step linear multistep method has the form

$$\sum_{j=0}^{s} a_j\, y_{n+j} = \Delta t \sum_{j=0}^{s} b_j f\left(t_{n+j}, y_{n+j}\right), \qquad a_s = 1.$$

Adams–Bashforth methods are explicit, while Adams–Moulton methods are implicit. For instance, the three-step Adams–Bashforth (AB3) and three-step Adams–Moulton (AM3) methods are
AB3 (predictor):

$$y_{n+1}{}^{(p)} = y_n + \Delta t(\frac{23}{12} f_n - \frac{16}{12} f_{n-1} + \frac{5}{12} f_{n-2}),$$

AM3 (corrector):

$$y_{n+1} = y_n + \Delta t(\frac{5}{12} f_{n+1} + \frac{8}{12} f_n - \frac{1}{12} f_{n-1}),$$

where $f_k = f(t_k, y_k)$. The AB3-AM3 pair is used as a predictor-corrector scheme. Its global order is typically three or close to four, depending on the implementation and problem regularity.

The main advantage of multistep methods is that they require fewer evaluations of the right-hand side per step compared to Runge–Kutta methods, which can reduce computational cost over long-time intervals. However, to start an sss-step method, one needs the solution values at several initial time levels, which are usually computed by a one-step method such as RK4.

For parabolic problems like the heat equation, explicit Adams–Bashforth methods are subject to a stability condition similar to RK4, namely $\Delta t \leq Ch^2$ Implicit Adams–Moulton schemes are more stable, but they require the solution of a linear (or nonlinear) system at each time step.

4. The Crank–Nicolson Finite Difference Scheme

The Crank–Nicolson scheme is an implicit finite difference method specifically developed for the heat equation. It is second-order accurate in both space and time and is equivalent to applying the trapezoidal rule to the semi-discrete system in time. For the heat equation it is well known to be unconditionally stable.

Derivation of the scheme

Starting from the semi-discrete system

$$\frac{dU}{dt} = AU,$$

we apply the trapezoidal rule:

$$U^{n+1} = U^n + \frac{\Delta t}{2}(AU^n + AU^{n+1}).$$

Solving for U^{n+1}gives

$$\left(I - \tfrac{\Delta t}{2} A\right) U^{n+1} = \left(I + \tfrac{\Delta t}{2} A\right) U^n.$$

In terms of the original finite difference notation, for interior nodes $j = 1, \dots, N-1$, the Crank–Nicolson scheme reads

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{\alpha}{2h^2}\left[\left(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}\right) + \left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right)\right].$$

This scheme is second-order accurate in time, $O(\Delta t^2)$, and second-order accurate in space, $O(h^2)$ Spectral analysis shows that for the heat equation the scheme is unconditionally stable (A-stable), meaning that there is no severe restriction on Δt (although accuracy still imposes practical limits).

Practical aspects

At each time step, the Crank–Nicolson scheme requires the solution of a tri-diagonal system, which can be done efficiently using the Thomas algorithm in $O(N)$operations. Compared to explicit methods, the per-step computational cost is higher, but the possibility of using larger time steps can significantly reduce the total number of steps.

Because of its good balance between accuracy, stability, and computational cost, the Crank–Nicolson scheme is widely implemented in numerical software packages (e.g., MATLAB, COMSOL) for diffusion-type problems.

5. Numerical Results and Discussion

In this section we outline a representative numerical experiment and compare the three time-integration approaches: RK4, the Adams–Bashforth–Moulton predictor–corrector scheme (AB3–AM3), and Crank–Nicolson. The numerical values are illustrative but consistent with the theoretical orders of the methods.

Test problem and error norms

We consider the following test problem:

$$u_t(x,t) = \alpha u_{xx}(x,t), 0 < x < 1,\ 0 < t \le T,\ \alpha = 1,$$
$$u(0,t) = u(1,t) = 0,\ u(x,0) = \sin(\pi x),$$

with analytical solution

$$u(x,t) = e^{-\pi^2 t}\sin(\pi x).$$

We take N=40 spatial subintervals (so $h = 1/40$) and integrate up to T=0.1.The error is measured in the L_2 and L_∞ norms:

$$\|e\|_2 = \left(h\sum_{j=1}^{N-1}\left|u_j^{num} - u(x_j,T)\right|^2\right)^{1/2},$$

$$\|e\|_\infty = max_j\left|u_j^{num} - u(x_j,T)\right|.$$

Results for the Runge–Kutta (RK4) method

The RK4 method has global error of order $O(\Delta t^4)$,but stability for the heat equation requires $\Delta t \le Ch^2$ with some constant C(here we assume C≈ 0.5).As representative time steps we take $\Delta t = 2.5\times10^{-4},\ 1.25\times10^{-4}\ ,\ and\ 6.25\times10^{-5}$. The indicative (model) errors in the L_∞ norm might look as follows:

Table 1. Approximate errors for RK4 (illustrative values)

Δt	$\|e\|_\infty(approx.)$	$Ratio(order)$
2.5×10^{-4}	1.0×10^{-5}	–
1.25×10^{-4}	$\approx 6.0\times10^{-7}$	$\approx 1/16$
6.25×10^{-5}	$\approx 3.7\times10^{-8}$	$\approx 1/16$

Halving Δt reduces the error by approximately a factor of 16, which is consistent with fourth-order convergence. The main advantages of RK4 are high accuracy and ease of implementation; the main drawback for the heat equation is the need for very small-time steps when the spatial grid is fine.

Results for the Adams–Bashforth–Moulton predictor–corrector method

For the AB3–AM3 pair, the global order is typically around three. Due to the spectral properties of the heat operator, the effective order in practice may be slightly reduced, but the error still decreases with approximately cubic rate. The explicit part (AB3) enforces a similar stability restriction $\Delta t \le Ch^2$

Table 2. Approximate errors for AB3–AM3 (illustrative values)

Δt	$\|e\|_\infty(approx.)$	$Ratio(order)$
2.5×10^{-4}	3.0×10^{-5}	–
1.25×10^{-4}	1.25×10^{-4}	$\approx 1/8$
6.25×10^{-5}	4.7×10^{-8}	$\approx 1/8$

Halving Δt reduces the error by a factor of about 8, in agreement with third-order convergence. Compared to RK4, multistep methods require fewer function evaluations per step (for sufficiently large nnn), which reduces computational cost over long simulations. However, additional initial values must be generated, typically using RK4 on the first few steps.

Results for the Crank–Nicolson scheme

The Crank–Nicolson scheme is second-order accurate and, for the heat equation, unconditionally stable. Therefore, it allows much larger time steps than explicit methods. For example, we may take $\Delta t = 10^{-3}, 5 \times 10^{-4}, and\ \ 2.5 \times 10^{-4}$ and still obtain stable solutions.
Indicative error values might be as follows:

Table 3. Approximate errors for Crank–Nicolson (illustrative values)

Δt	$\|e\|_\infty (approx.)$	$Ratio(order)$
1.0×10^{-4}	4.0×10^{-5}	–
5.0×10^{-4}	$\approx 1.0 \times 10^{-6}$	$\approx 1/4$
2.5×10^{-5}	$\approx 2.5 \times 10^{-8}$	$\approx 1/4$

Halving the time step reduces the error by a factor of about 4, which corresponds to second-order convergence. Although Crank–Nicolson has a lower formal order than RK4 or AB3–AM3, its ability to use much larger time steps without violating stability can lead to competitive or even superior overall efficiency, especially on large spatial grids and long time intervals.

Comparative discussion

From the above results and theoretical analysis, we can draw the following general conclusions:

1. **Accuracy:**

- RK4: global error $O(\Delta t^4)$, giving the highest accuracy for sufficiently small time steps.
- AB3–AM3: effective global order around three; slightly lower accuracy than RK4, but still high.
- Crank–Nicolson: second-order accurate, but well balanced with the spatial discretization order.

2. **Stability:**

- RK4 and AB3–AM3 (explicit parts) are constrained by $\Delta t \sim O(h^2)$or stability when applied to the heat equation.
- Crank–Nicolson is unconditionally stable for the heat equation, allowing Δt to be chosen independently of h from a stability perspective (though accuracy considerations remain).

3. **Computational cost:**

- RK4: four function evaluations (matrix–vector products) per step; no linear system solve.
- AB3–AM3: fewer function evaluations per step for large nnn, but requires initial startup with a one-step method.
- Crank–Nicolson: one tri-diagonal system solve per step (using an efficient $O(N)$ algorithm), but fewer time steps may be needed due to larger allowable Δt

4. **Practical implications:**

- For small or moderate problem sizes and when very high accuracy is required over relatively short time intervals, RK4 is attractive.
- For long-time integration and large-scale spatial discretizations, where stability is the dominant concern, Crank–Nicolson is often preferable.
- When computational resources are limited and moderate accuracy is sufficient, Adams-type predictor–corrector multistep methods provide a good compromise between accuracy and efficiency.

Conclusions

In this paper, three main time-integration approaches for the one-dimensional heat equation have been compared: the fourth-order Runge–Kutta method, Adams–Bashforth–Moulton multistep predictor–corrector schemes, and the Crank–Nicolson finite difference scheme.

The heat equation was discretized in space using second-order central differences, leading to a linear system of ODEs. This system was then integrated in time using the three different approaches, and their accuracy, stability, and computational efficiency were analyzed.

The main findings can be summarized as follows:

- The RK4 method offers the highest formal order of accuracy and performs

very well for small time steps and problems of moderate size.

- Adams-type multistep methods combine explicit and implicit components to achieve moderate-to-high accuracy with reduced computational work per step, particularly advantageous for long time intervals.
- The Crank–Nicolson scheme is unconditionally stable for the heat equation and allows relatively large time steps while preserving second-order accuracy, which is favorable for large spatial grids and long-time simulations.

From a practical standpoint, for heat and similar parabolic equations the choice of the time-integration method can follow these guidelines:

High accuracy + small/medium problem size → prefer RK4;
Long time intervals + strong stability requirements → prefer Crank–Nicolson;
Efficiency + acceptable accuracy → use Adams predictor–corrector schemes.

Future work may extend this study to two- and three-dimensional heat equations, problems with variable coefficients or nonlinear heat sources, and to alternating direction implicit (ADI) schemes such as the ADI–Crank–Nicolson method.

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