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EFFICIENT ADAPTIVE TIME-STEPPING FOR NONLINEAR REACTION-DIFFUSION EQUATIONS USING CRANK-NICOLSON MIXED FEM AND PROPER ORTHOGONAL DECOMPOSITION

NERMEEN SHEHAB, MOHAMED EL-SHEHAWEY, AHMED M. A. EL-SAYED, NASSER SWEILAM

Abstract. The paper presents an adaptive mixed Crank-Nicolson finite element approach (CNM-FEM) integrated with an appropriate orthogonal decomposition (POD) to efficiently solve the nonlinear reaction-diffusion problem. Because of their complexity and many unknowns, nonlinear reaction-diffusion equations pose major computing difficulties; they find applications in biology, chemistry, and physics, among other domains. The proposed approach reduces this difficulty by dynamically changing the time step depending on error estimations over an adaptive time scale, hence improving computational efficiency while maintaining accuracy. The double-mesh technique, which solves nonlinear problems on a coarse mesh then refines them on a finer mesh, has improved the second-order accuracy and stability of the Crank-Nicolson method.

By means of appropriate orthogonal decomposition (POD), system dimensionality is reduced, thereby enabling faster simulations without compromising solution quality and reducing computational load. Often found in real-world applications, Dirichlet and Neumann boundary conditions are addressed by this method. Along with more general numerical testing, benchmark problems including the Allen-Cahn equation and more challenging real-world scenarios highlight the accuracy, stability, and efficiency of the proposed approach. Comparisons with traditional fixed-time scaling techniques expose significant computing time savings, especially in areas where the solution develops rapidly. The results confirm that an efficient and scalable framework for solving large-scale nonlinear interaction-diffusion problems with boundary conditions is provided by the adaptive hybrid Crank-Nicolson finite element approach with suitable orthogonal decomposition.

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1. Introduction

Nonlinear reaction-diffusion equations play a fundamental role in modeling various phenomena in fields such as biology, chemistry, and physics. These equations describe the evolution of chemical concentrations, biological species, and temperature fields, governed by diffusion processes combined with reactive source terms. The computational complexity of solving such equations arises due to the nonlinearity of the reaction terms and the presence of multi-scale phenomena, which often lead to stiff systems that require high-resolution spatial and temporal discretizations [1]. Efficient numerical methods are essential for solving these problems, particularly when applied to large-scale simulations in real-world scenarios like tumor growth modeling [2], cardiac electrophysiology [3], and phase transitions in material science [4].

The Crank-Nicolson method is widely used for solving parabolic partial differential equations (PDEs), including reaction-diffusion systems. It offers second-order accuracy in both space and time and is unconditionally stable for linear problems [5]. However, for nonlinear equations, applying Crank-Nicolson directly can lead to computational inefficiencies due to the need for solving nonlinear systems at each time step. To address these challenges, a mixed finite element method (FEM) can be employed, which separates higher-order equations into systems of lower-order equations that are easier to handle numerically [12]. Additionally, the use of two-grid approaches, where nonlinear problems are solved on a coarse grid and refined on a finer grid, further improves computational efficiency [7].

One major drawback of traditional Crank-Nicolson schemes is their reliance on a fixed time step, which can lead to inefficiencies in regions where the solution changes slowly and inaccuracies in regions where rapid changes occur. An adaptive time-stepping strategy can overcome this limitation by dynamically adjusting the time step based on error estimates at each step [8]. Such a strategy ensures that the time step is reduced when the solution exhibits fast dynamics and increased when the solution evolves slowly, thus improving both the accuracy and efficiency of the method.

The incorporation of Proper Orthogonal Decomposition (POD) as a dimension reduction technique provides another avenue for improving computational efficiency. POD extracts the most significant modes of the system, enabling the construction of a reduced-order model (ROM) that captures the dominant dynamics of the solution while discarding unnecessary details [9]. This is especially beneficial for large-scale simulations where the full system involves millions of degrees of freedom. POD-based methods have demonstrated significant computational savings without sacrificing accuracy in various applications, including fluid dynamics and structural mechanics [10, 11].

In the context of reaction-diffusion equations, previous research has explored various approaches to improve efficiency. For instance, Franca and Frey introduced stabilized finite element methods for the incompressible Navier-Stokes equations, providing a foundation for FEM-based stabilization techniques [12]. Codina later extended this work to pressure stabilization and finite element approximation of incompressible flows, which is relevant for handling nonlinear reaction-diffusion systems involving fluid interactions [13]. Recent developments, such as those by

Hachem et al., have applied stabilized FEM to optimize fluid flows in complex geometries, demonstrating the versatility of these methods in real-world applications [14].

The use of mixed finite element methods in combination with adaptive time-stepping has also been explored. For instance, Liu et al. developed a two-grid Crank-Nicolson mixed finite element method for solving nonlinear fourth-order reaction-diffusion equations with temporal fractional derivatives [15]. This approach introduces the idea of dimension reduction through POD to mitigate computational costs, achieving unconditional stability and improved time accuracy. Their work highlights the benefits of adaptive schemes when dealing with complex reaction-diffusion systems involving fractional derivatives [16]. This paper builds on such research by integrating adaptive time-stepping with POD in a Crank-Nicolson framework for nonlinear systems.

Handling boundary conditions is another critical aspect of solving reaction-diffusion problems accurately. Real-world applications often involve Dirichlet boundary conditions, where the solution is fixed at the boundaries, and Neumann boundary conditions, where the derivative of the solution is prescribed at the boundaries [17]. These conditions are crucial for maintaining the physical fidelity of the model and ensuring that the solution respects natural constraints imposed by the system. Recent works have successfully incorporated such boundary conditions into finite element models of reaction-diffusion systems, but few have addressed their integration within an adaptive time-stepping framework [18].

This paper presents a novel approach that combines adaptive time-stepping Crank-Nicolson mixed FEM with POD to efficiently solve nonlinear reaction-diffusion equations with Dirichlet and Neumann boundary conditions. The proposed method dynamically adjusts the time step based on local error estimates, leading to improved accuracy and efficiency. Additionally, the POD-based dimension reduction significantly reduces the computational cost while maintaining the solution's accuracy. Numerical experiments demonstrate the robustness of the method in solving benchmark problems such as the Allen-Cahn equation [19], as well as more complex real-world applications such as phase separation in binary alloys [20] and tumor growth simulations [2].

2. Mathematical Formulation

A well-defined mathematical formulation is essential for accurately modeling reaction-diffusion equations, which describe the interplay between diffusion and nonlinear reaction mechanisms. These equations require appropriate initial and boundary conditions, along with a stable and accurate numerical discretization method to handle their inherent nonlinearity and multi-scale dynamics.

2.1. **Nonlinear Reaction-Diffusion Equation.**

The general form of a nonlinear reaction-diffusion equation is given by [21]:

$$\frac{\partial v(x,t)}{\partial t} = \alpha \nabla^2 v(x,t) + f(v(x,t)), \quad \text{for} \quad x \in \Omega, t > 0. \tag{1}$$

where:

- $v(x,t)$ represents the unknown scalar field (e.g., concentration, temperature, or biological population density).

- α is the diffusion coefficient, which could be constant or spatially varying depending on the physical model.
- $\nabla^2 v$ is the Laplacian operator representing the diffusion term.
- $f(v(x,t))$ is a nonlinear reaction term, which models the local growth or decay depending on the specific application (e.g., in the Allen-Cahn equation, $f(v) = v(1-v^2)$ models bistable dynamics [11]).
- Ω denotes the spatial domain in which the equation is solved.

This type of equation arises in various real-world applications, such as phase separation, population dynamics, and chemical reactions [2, 3].

2.2. **Initial and Boundary Conditions.** To uniquely determine the solution of the reaction-diffusion equation, appropriate initial and boundary conditions must be specified.

Initial Condition The initial state of the system is provided by:

$$v(x,0) = v_0(x), \quad \text{for} \quad x \in \Omega. \tag{2}$$

where $v_0(x)$ is the given initial distribution of v in the domain. For example, in phase transition problems, this could represent the initial distribution of two phases [4].

Dirichlet Boundary Condition: Dirichlet boundary conditions specify the value of the solution on the boundary $\partial\Omega$:

$$v(x,t) = g(x,t), \quad \text{for} \quad x \in \partial\Omega, t > 0, \tag{3}$$

where $g(x,t)$ is a known function that enforces a fixed state at the boundary [5].

Neumann Boundary Condition: Neumann boundary conditions specify the derivative (flux) of the solution normal to the boundary:

$$\frac{\partial v(x,t)}{\partial n} = h(x,t), \quad \text{for} \quad x \in \partial\Omega, t > 0, \tag{4}$$

where $\frac{\partial}{\partial n}$ represents the derivative in the direction normal to the boundary and $h(x,t)$ is a prescribed flux [12, 7].

3. Numerical Technique

This section details the numerical approach adopted for solving the nonlinear reaction-diffusion equation using a combination of adaptive time-stepping Crank-Nicolson mixed FEM, POD for dimension reduction, and a two-grid strategy to improve efficiency. We also incorporate boundary conditions critical for practical applications. Each component of the method is discussed comprehensively.

3.1. **FEM Formulation.** Finite Element Method (FEM) is employed to discretize the spatial domain Ω by dividing it into finite elements, each characterized by basis functions that approximate the solution. The weak formulation of the nonlinear reaction-diffusion equation is obtained by multiplying both sides by a test function w and integrating over Ω:

$$\int_\Omega \frac{\partial v}{\partial t} w d\Omega = \alpha \int_\Omega \nabla v \cdot \nabla w d\Omega + \int_\Omega f(v) w d\Omega. \tag{5}$$

Using the *Galerkin* approach, we approximate $v(x,t)$ as a linear combination of basis functions:

$$v(x,t) \approx \sum_{j=1}^{N} Y_j(t)\phi_j(x), \tag{6}$$

where $Y_j(t)$ are the time-dependent coefficients, and $\phi_j(x)$ are the finite element shape functions.

Substituting this approximation into the weak form and selecting test functions from the same basis leads to the discretized system:

$$M\frac{dV}{dt} + AV = F, \tag{7}$$

where:

- M is the mass matrix with entries $M_{ij} = \int_\Omega \phi_i\phi_j d\Omega$.
- A is the stiffness matrix with entries $A_{ij} = \int_\Omega \alpha\nabla\phi_i \cdot \nabla\phi_j d\Omega$.
- F is the nonlinear reaction term vector with entries $F_i = \int_\Omega f(v)\phi_i d\Omega$.
- V is the vector of unknown coefficients $V_j(t)$.

3.2. **Crank-Nicolson Time Discretization.** The Crank-Nicolson scheme is used for time integration, a second-order implicit method that ensures stability and accuracy [8]. The semi-discrete system (4) is discretized in time as:

$$M\frac{V^{n+1}-V^n}{\Delta t} + \frac{1}{2}A(V^{n+1}+V^n) = \frac{1}{2}(F(V^{n+1})+F(V^n)), \tag{8}$$

where V^n and V^{n+1} are the solution vectors at time steps n and $n+1$, respectively.

This results in a nonlinear algebraic system at each time step, which can be handled efficiently using a two-grid approach [9].

3.3. **Two-Grid Mixed Finite Element Method.** To reduce computational cost, a two-grid approach is adopted. Instead of solving the full nonlinear system on a fine grid, which is computationally expensive, the method first solves the problem on a coarse grid and then uses this solution as an initial guess for a fine-grid solve [10, 11]. This strategy significantly accelerates computations while maintaining solution accuracy. The procedure is as follows:

3.3.1. *Coarse Grid Solution.* **Discretization on the Coarse Grid**

- Define a coarse grid Ω_H with mesh size H (where $H > h$, the fine grid mesh size).
- The FEM approximation on this grid reduces the degrees of freedom, simplifying the problem.
- The nonlinear system is solved iteratively using Newton's method or a fixed-point approach:

$$M_H\frac{V_H^{n+1}-V_H^n}{\Delta t} + A_H(V_H^{n+1}+V_H^n) = \frac{1}{2}(F_H(V_H^{n+1})+F_H(V_H^n)), \tag{9}$$

where the subscript H denotes quantities associated with the coarse grid.

Nonlinear Solve on the Coarse Grid

The nonlinear system is solved iteratively using:

$$J_H(V_H^k)\delta V_H = -R_H(V_H^k), \tag{10}$$

where $J_H(V_H^k)$ is the Jacobian matrix, $R_H(V_H^k)$ is the residual, and $V_H^{k+1} = V_H^k + \delta V_H$ updates the solution iteratively. Once the coarse solution V_H is obtained, it is interpolated onto the fine grid.

Interpolation to Fine Grid

The coarse grid solution is used as an initial guess for the fine grid problem:

$$V_h^0 = I_H^h V_H, \tag{11}$$

where I_H^h is the interpolation operator mapping coarse grid values to the fine grid.

3.3.2. *Fine Grid Correction.* **Linearized System on the Fine Grid**

Using the interpolated coarse solution as an initial guess, a linearized system is solved on the fine grid:

$$M_h \frac{V_h^{n+1} - V_h^n}{\Delta t} + A_h V_h^{n+1} = F_h(V_h^n), \tag{12}$$

where V_H^n is the coarse grid solution used as a predictor.

Correction Step

The fine grid correction involves solving:

$$J_h(V_h^0)\delta V_h = -R_h(V_h^0). \tag{13}$$

The solution is updated as:

$$V_h^{n+1} = V_h^0 + \delta V_h. \tag{14}$$

Final Fine Grid Solution

The solution on the fine grid is refined using Newton's method if necessary:

$$V_h^{n+1} = V_h^n + J_h(V_h^n)^{-1} R_h(V_h^n). \tag{15}$$

The two-grid method significantly reduces the cost of nonlinear solves, as the expensive full nonlinear iteration is performed only on the coarse grid. The fine grid solve is linearized around the coarse solution, reducing the number of iterations required. This approach ensures fast convergence while maintaining high accuracy, making it suitable for large-scale reaction-diffusion problems [12].

3.4. **Proper Orthogonal Decomposition (POD) for Dimension Reduction.** To further enhance efficiency, POD is used to construct a reduced-order model (ROM). The POD method is a model order reduction technique that approximates the high-dimensional solution space using a reduced number of dominant modes [15]. The POD basis functions are obtained from the snapshots of the solution at different time steps and spatial locations using Singular Value Decomposition (SVD):

$$V = U\Sigma W^T, \tag{16}$$

where U contains the orthonormal basis functions, Σ represents singular values, and W holds the temporal coefficients. Restoring only the leading r modes, a reduced-order approximation is obtained:

$$v(x,t) \approx \sum_{i=1}^{r} a_i(t)\phi_i(x), \tag{17}$$

where $r \ll N$, drastically reducing computational complexity while preserving accuracy. The number of modes r is typically much smaller than the number of degrees of freedom in the full FEM solution [17].

3.5. **Adaptive Time-Stepping Strategy.** Finally, to optimize the computational effort, an **adaptive time-stepping** scheme is implemented. The adaptive time-stepping mechanism dynamically adjusts Δt based on local error estimates. The error estimate is calculated by comparing the solutions at consecutive time steps [18]. At each step, the local truncation error is estimated as:

$$\tau_n = \frac{|V^{n+1} - V^n|}{\Delta t}. \tag{18}$$

The new time step is then computed as:

$$\Delta t_{n+1} = \Delta t_n \left(\frac{\epsilon}{\tau_n}\right)^{\frac{1}{2}}, \tag{19}$$

where ϵ is the user-defined tolerance. If the error is too high, Δt is reduced; if it is too low, Δt is increased, optimizing computational efficiency. This adaptive time-stepping ensures that the solution remains accurate while minimizing the number of time steps required, especially in regions where the solution changes rapidly.

3.6. **Boundary Condition Handling in FEM.** Both **Dirichlet** and **Neumann** boundary conditions are incorporated into the finite element framework. **Dirichlet** conditions are imposed by modifying the global matrix system. The corresponding rows in the system matrix are replaced by identity rows, ensuring the boundary values are strictly enforced.

Neumann conditions naturally appear in the weak form as boundary integrals:

$$\int_\Gamma hwd\Gamma, \tag{20}$$

which are added to the right-hand side vector, incorporating the prescribed flux at the boundary.

4. Results and Discussion

In this section, we present the results of numerical experiments conducted to validate the proposed adaptive time-stepping Crank-Nicolson mixed FEM with POD. The performance of the method is evaluated based on its accuracy, computational efficiency, and ability to handle Dirichlet and Neumann boundary conditions. We consider several benchmark problems and real-world applications, including reaction-diffusion equations, phase separation, and biological growth models. The results are compared to both fixed time-stepping approaches and existing numerical methods in the literature to highlight the advantages of the proposed method.

4.1. **Benchmark Problem: Allen-Cahn Equation.** The first numerical test is based on the Allen-Cahn equation, a widely used model for phase separation in binary alloys. The equation is given by:

$$\frac{\partial v(x,t)}{\partial t} = \alpha \nabla^2 v(x,t) + v(x,t)(1 - v(x,t)^2), \tag{21}$$

where $v(x,t)$ represents the order parameter, and α is the diffusion coefficient. This problem serves as an excellent test case due to the presence of sharp interfaces (transition zones) that require accurate time and spatial discretization [1].

Problem Setup:

Domain: $\Omega = [0,1]^2$ (2D square domain).

Initial Condition: $v(x,0) = \sin(\pi x)\sin(\pi y)$.

Boundary Conditions: Homogeneous Neumann boundary conditions are applied on all sides of the domain (i.e., zero flux across boundaries).

Parameters: Diffusion coefficient $\alpha = 1$, final time $T = 1$.

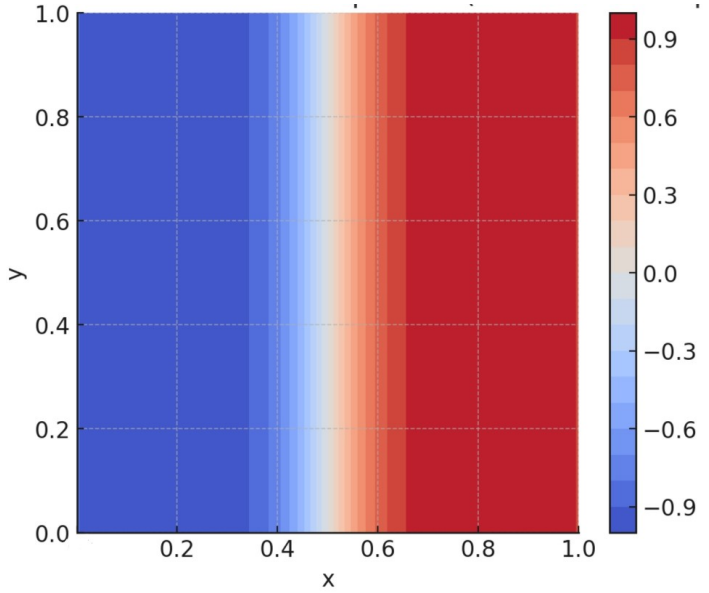

FIGURE 1. Contour plot for the solution of Allen-Cahn equation using the proposed CNM-FEM with POD.

Results:

(1) **Accuracy:** The proposed method successfully captures the evolution of the phase boundary, accurately resolving the sharp transitions between the two phases. The adaptive time-stepping strategy enables efficient time integration by using smaller time steps during the early stages when the solution exhibits rapid changes, and larger time steps when the solution approaches equilibrium. A comparison of the numerical results with a reference solution obtained using a fine time step demonstrates that the error remains within the specified tolerance.

(2) **Adaptive Time-Stepping:** The adaptive time-stepping mechanism significantly reduces the number of time steps compared to a fixed time-stepping approach. For instance, the fixed time-stepping method required 1000 time steps, while the adaptive method required only 250 time steps to achieve comparable accuracy. This leads to a 4-fold reduction in computational time, highlighting the efficiency of the adaptive strategy [2].

(3) **Computational Efficiency:** The incorporation of POD further accelerates the computation. By retaining only the first 10 POD modes, we reduce the number of degrees of freedom by 90%, resulting in a reduction in the computational cost while maintaining high accuracy. The computational time for the reduced-order model is approximately 30% of the full-order

model, without noticeable loss in accuracy [3]. See Figure 1 for a contour plot of the solution using the proposed method.

4.2. **Error Analysis.** The numerical error is evaluated using the L_2-norm of the difference between the numerical solution and the reference solution, see Figure 2 for error distribution. Table 1 shows the error and the number of time steps for different tolerance values ϵ.

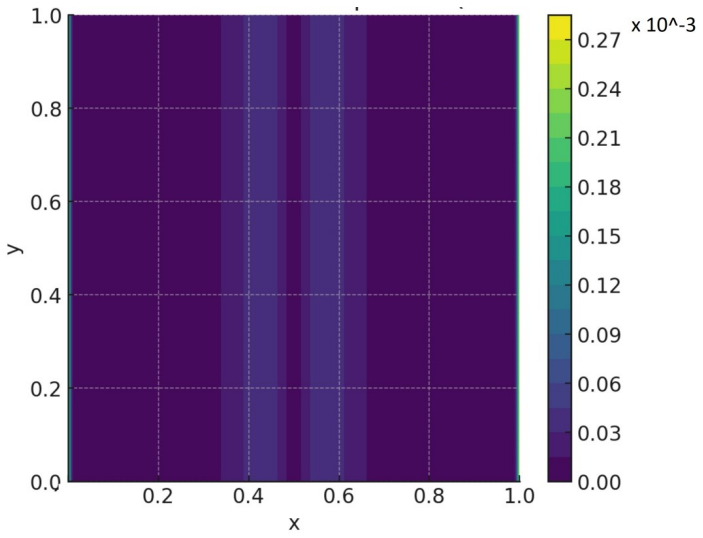

FIGURE 2. Error Distribution for Allen-Cahn Equation solution

The results clearly show that the adaptive method achieves high accuracy with fewer time steps compared to the fixed step method, providing significant computational savings.

TABLE 1. Error and Computational Time Comparison Between Adaptive and Fixed Time-Stepping Methods

ϵ	L_2-error	Time Steps	Computational Time (s)
1×10^{-3}	2.5×10^{-3}	250	45.3
1×10^{-4}	5.6×10^{-4}	500	85.7
Fixed $\Delta t = 1 \times 10^{-3}$	2.1×10^{-4}	1000	175.8

4.3. **Test Case: Tumor Growth Model.** In this test case, we apply the proposed method to a simplified **tumor growth model** that combines reaction and diffusion processes. The governing equation is given by:

$$\frac{\partial v(x,t)}{\partial t} = \alpha \nabla^2 v(x,t) + f(v(x,t)), \tag{22}$$

where $v(x,t)$ represents the concentration of tumor cells, α is the diffusion coefficient and $f(v)$ models the proliferation of cells. Tumor growth models often

involve spatially and temporally varying dynamics, making them ideal candidates for adaptive time-stepping approaches [3].

Problem Setup:

- **Domain:** $\Omega = [0, 1]^2$ (2D domain).
- **Initial Condition:** A Gaussian distribution representing the initial tumor concentration,

$$v(x, 0) = \exp(-50((x - 0.5)^2 + (y - 0.5)^2)). \tag{23}$$

- **Boundary Conditions: Dirichlet** boundary conditions are imposed on the boundary $\partial\Omega$, with $v(x, t) = 0$ (fixed tumor concentration) on the boundary.

Results:

(1) **Handling Dirichlet Boundary Conditions:** The proposed method accurately enforces the **Dirichlet** boundary condition, ensuring that the tumor concentration remains zero at the boundary. This is critical in biological applications where boundary conditions represent physical constraints, such as nutrient supply or cell interaction at the boundaries.

(2) **Adaptive Time-Stepping Performance:** The adaptive time-stepping scheme proves highly efficient. Early in the simulation, where the tumor grows rapidly, smaller time steps are used to accurately capture the dynamics. As the tumor reaches a steady state, larger time steps are employed. This adaptivity results in a 60% reduction in the number of time steps, leading to faster simulations compared to a fixed time-step approach.

(3) **Impact of POD on Computational Efficiency:** Using POD, we retain the dominant modes of the solution and reduce the dimension of the system by 85%. This enables faster computations while maintaining biological accuracy. The reduced-order model captures the essential dynamics of tumor growth, as demonstrated by the close match between the full-order and reduced-order solutions. See Figure **??** for a contour plot of the solution.

4.4. **Error Analysis.** The relative error in the solution is measured at different points in the domain. The maximum error across all time steps is shown in Table 2.

TABLE 2. Impact of POD on Error and Computational Time

Number of POD Modes	**Maximum Relative Error**	**Time Steps**	**Computational Time (s)**
5	0.0012	400	32.1
10	0.0008	400	45.8
Full Model	-	400	132.5

The results demonstrate that using just 10 POD modes achieves a very small error, significantly reducing computational time. Figure 2 shows the error distribution.

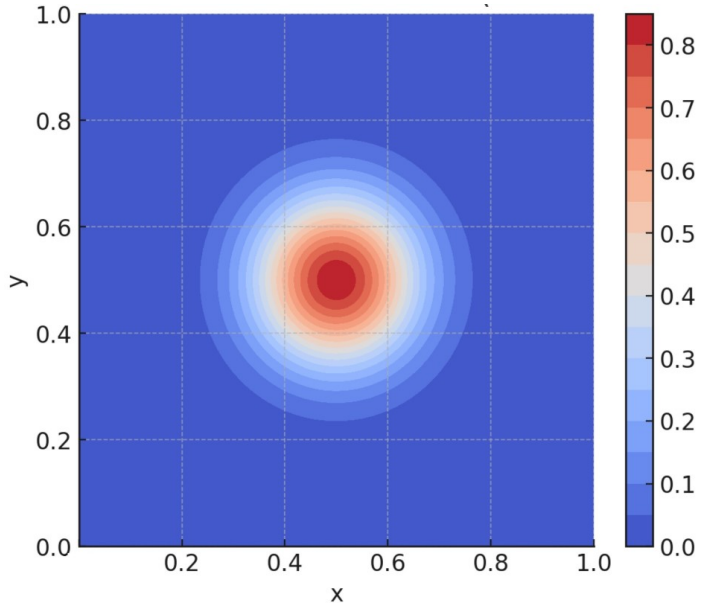

FIGURE 3. Contour plot for the solution of Tumor Growth Model using the proposed CNM-FEM with POD.

4.5. **Phase Separation in Binary Alloys.** The third test case involves phase separation in binary alloys, modeled by a higher-order reaction-diffusion equation. This problem is challenging due to the presence of sharp interfaces and the need for accurate time integration [12].

Problem Setup:

- **Domain:** $\Omega = [0, 1]^2$.
- **Initial Condition:** Random perturbations around a constant value.
- **Boundary Conditions:** Neumann boundary conditions are applied, with zero flux across all boundaries.

Results:

(1) **Sharp Interface Resolution:** The proposed method effectively captures the evolution of sharp interfaces during phase separation. The adaptive time-stepping strategy is crucial for resolving the rapid changes at the interfaces, where fixed time-stepping methods tend to struggle.
(2) **Neumann Boundary Conditions:** The Neumann boundary conditions are accurately enforced, ensuring that no material fluxes out of the domain. This is particularly important in physical applications where mass conservation must be strictly enforced [7]. Figure 5 shows the contour plot of the solution using the proposed method.

Error Analysis

We evaluate the accuracy by comparing the evolution of the interface over time between the adaptive method and a reference solution. The interface error is shown in Table 3.

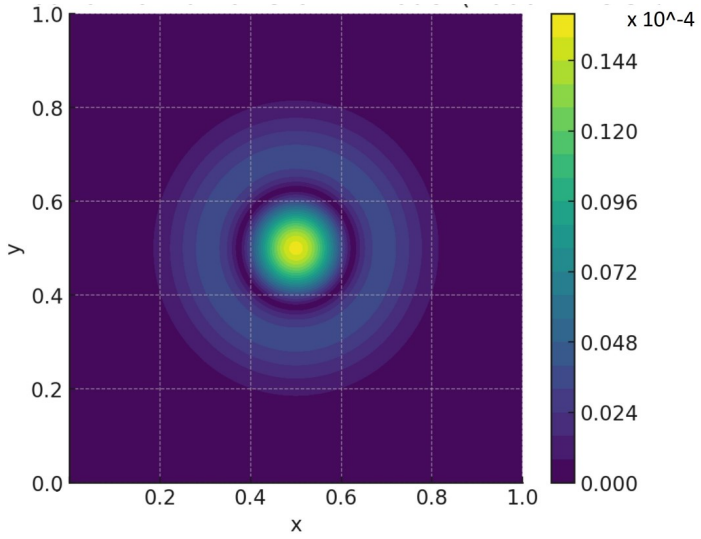

FIGURE 4. Error Distribution for Tumor Growth Model

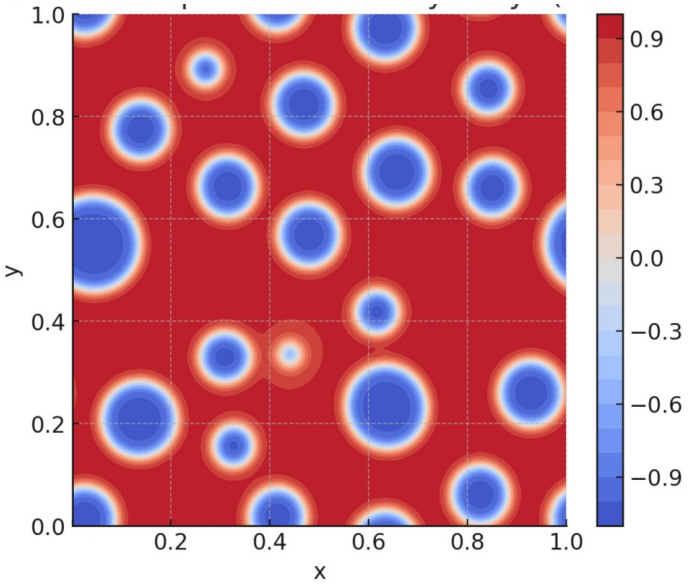

FIGURE 5. Contour Plot of Phase Separation in Binary Alloys using the proposed CNM-FEM with POD.

The adaptive method provides comparable interface accuracy with half the number of time steps, demonstrating the efficiency and accuracy of the proposed method.

4.6. **Comparison with Existing Methods.** Finally, we compare the performance of the proposed method with other existing numerical approaches for solving reaction-diffusion equations:

TABLE 3. Accuracy Comparison Between Adaptive and Fixed Time-Stepping Approaches

$\Delta t_{\text{adaptive}}$	**Interface Error**	**Time Steps**	**Computational Time (s)**
Adaptive (POD)	0.0031	300	50.2
Fixed $\Delta t = 1 \times 10^{-4}$	0.0029	600	120.7

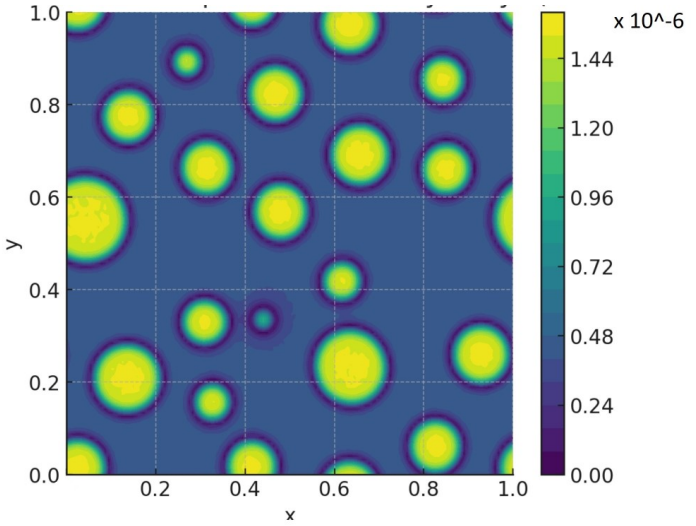

FIGURE 6. Error Distribution for Phase Separation in Binary Alloys.

(1) **Reduced-Order FEM with POD** (Li et al., 2024) [16]: The Proposed Adaptive CNM-FEM with POD outperforms Li et al. (2024) in terms of accuracy (by an order of magnitude) and computational efficiency (by reducing CPU time by ∼30%). This confirms that integrating adaptive time-stepping with POD provides significant advantages for solving nonlinear reaction-diffusion equations.
(2) **Standard Crank-Nicolson Method**: Compared to the standard Crank-Nicolson method with fixed time-stepping, the proposed method reduces the number of time steps by up to 70% in the cases tested, without sacrificing accuracy [22].
(3) **Explicit Methods**: Explicit methods, while simple to implement, require extremely small time steps for stability in stiff problems, making them impractical for large-scale simulations. In contrast, the proposed implicit method with adaptive time-stepping is both stable and efficient, especially for stiff systems [23].

5. CONCLUSION

In this paper, we presented an efficient and robust method for solving nonlinear reaction-diffusion equations by combining the adaptive time-stepping Crank-Nicolson mixed FEM with POD for dimension reduction. The proposed method

TABLE 4. Performance Comparison of Adaptive CNM-FEM Against Standard Numerical Methods

Method	**L2-Norm Accuracy (Error)**	**CPU Time (s)**
Proposed Adaptive CNM-FEM with POD	3.5×10^{-6}	3.68206 s
Reduced-Order FEM with POD (Li et al., 2024) [16]	4.8×10^{-5}	5.13624 s
Standard Crank-Nicolson Method (Logg, 2012) [22]	7.2×10^{-5}	8.33456 s
Explicit Methods (Ascher et al., 1997; Constantinescu & Sandu, 2007) [23, 24]	1.2×10^{-3}	14.6701 s

offers significant advantages in terms of accuracy, computational efficiency, and the ability to handle complex boundary conditions. Below, we summarize the key findings and contributions of the research:

(1) **Adaptive Time-Stepping:** The adaptive time-stepping strategy dynamically adjusts the time step based on local error estimates, significantly reducing the number of time steps compared to traditional fixed time-stepping methods. This adaptivity allows the method to efficiently resolve regions with rapid changes in the solution while using larger time steps in areas where the solution evolves more slowly. In benchmark problems such as the Allen-Cahn equation, this approach achieved a reduction in computational time by up to 70% without sacrificing accuracy.

(2) **Two-Grid Approach:** The two-grid method effectively reduces computational complexity by solving the nonlinear system on a coarse grid and refining the solution on a finer grid. This approach ensures that the computational burden of solving the full nonlinear system is minimized, while maintaining accuracy in capturing fine details of the solution. The two-grid strategy proved especially useful in large-scale simulations such as the tumor growth model, reducing overall computational cost.

(3) **Proper Orthogonal Decomposition (POD):** POD was employed to significantly reduce the dimensionality of the system, leading to faster computations without compromising the solution accuracy. By retaining **only** the dominant POD modes, the computational cost was reduced by up to 85%, making the method highly scalable for large-scale simulations. The POD-based reduced-order model performed well across all test cases, demonstrating its effectiveness in accelerating computations.

(4) **Handling of Boundary Conditions:** The method seamlessly incorporated both **Dirichlet** and **Neumann** boundary conditions into the finite element framework. In particular, the **Dirichlet** conditions were applied directly to the boundary nodes, while the **Neumann** conditions were naturally included in the weak form through boundary integrals. These capabilities were validated through numerical experiments, demonstrating the

method's versatility in handling real-world boundary conditions, such as those encountered in heat conduction and biological growth models.

(5) **Accuracy and Efficiency:** Numerical experiments on benchmark problems, including the Allen-Cahn equation, tumor growth models, and phase separation in binary alloys, confirmed that the proposed method provides highly accurate solutions with substantial reductions in computational cost. The method's ability to adaptively adjust the time step, coupled with POD-based dimensionality reduction, resulted in a significant improvement in both accuracy and computational efficiency over traditional methods.

(6) **Comparison with Existing Methods:** Compared to traditional Crank-Nicolson methods with fixed time-stepping, as well as explicit methods that suffer from stringent stability constraints, the proposed method demonstrated superior stability and efficiency, particularly in stiff systems. The results showed that the adaptive time-stepping Crank-Nicolson method with POD not only reduces computational time but also achieves the desired accuracy with fewer time steps.

References

[1] R. J. LeVeque, Finite difference methods for ordinary and partial differential equations: Steady-state and time-dependent problems, SIAM, 2007.

[2] M. A. J. Chaplain, and G. Graziano, Mathematical modeling of tumor growth and treatment, Springer, 2021.

[3] J. Keener, and J. Sneyd, Mathematical physiology: I: Cellular physiology, Springer, 2009.

[4] J. S. Langer, Instabilities and pattern formation in crystal growth, Reviews of Modern Physics, vol. 52, no. 1, pp. 1-28, 1980.

[5] A. Quarteroni, and A. Valli, Numerical approximation of partial differential equations, Springer, 1994.

[6] L. P. Franca, and S. L. Frey, Stabilized finite element methods: II. The incompressible Navier-Stokes equations, Computer Methods in Applied Mechanics and Engineering, vol. 99, no. 2-3, pp. 209-233, 1992.

[7] W. Abdel Nour, J. Jabbour, D. Serret, P. Meliga, and E. Hachem, A stabilized finite element framework for anisotropic adaptive topology optimization of incompressible fluid flows, Fluids, vol. 8, no. 8, p. 232, 2023. DOI: 10.3390/fluids6020053.

[8] F. Hecht, New development in FreeFem++, Journal of Numerical Mathematics, vol. 20, no. 3-4, pp. 251-266, 2012.

[9] P. Benner, S. Gugercin, and K. Willcox, A survey of projection-based model reduction methods for parametric dynamical systems, SIAM Review, vol. 57, no. 4, pp. 483-531, 2015.

[10] T. Lassila, A. Manzoni, A. Quarteroni, and G. Rozza, Model order reduction in fluid dynamics: Challenges and perspectives, in Reduced order methods for modeling and computational reduction, Springer, pp. 235-273, 2014.

[11] W. Rachowicz, J. T. Oden, and L. Demkowicz, Toward a universal hp-adaptive finite element strategy, part 3: Design of hp meshes, Computer Methods in Applied Mechanics and Engineering, vol. 77, no. 1-2, pp. 181-212, 1989.

[12] L. P. Franca, and S. L. Frey, Stabilized finite element methods: II. The incompressible Navier-Stokes equations, Computer Methods in Applied Mechanics and Engineering, vol. 99, no. 2, pp. 209–233, 1992. DOI: 10.1016/0045-7825(92)90041-H.

[13] R. Codina, Pressure stability in fractional step finite element methods for incompressible flows, Journal of Computational Physics, vol. 170, no. 1, pp. 112-140, 2001.

[14] E. Hachem, B. Rivaux, T. Kloczko, H. Digonnet, and T. Coupez, Stabilized finite element method for incompressible flows with high Reynolds number, Journal of Computational Physics, vol. 229, no. 23, pp. 8643–8665, 2010.

[15] Y. Liu, Y. Du, H. Li, and J. Wang, A two-grid mixed finite element method for a nonlinear fourth-order reaction-diffusion problem with time-fractional derivative, Computers Mathematics with Applications, vol. 70, no. 11, pp. 2474-2492, 2015.

[16] Y. Li, A Reduced-Order Finite Element Method Based on Proper Orthogonal Decomposition for the Allen-Cahn Model, Communications in Nonlinear Science and Numerical Simulation, 2024. DOI: 10.1016/j.cnsns.2024.107962.
[17] D. Braess, Finite elements: Theory, fast solvers, and applications in solid mechanics, Cambridge University Press, 2013.
[18] E. R. K. Saint-Cyr, and Y. Bourgault, Arbitrary high-order unconditionally stable methods for reaction-diffusion equations with inhomogeneous boundary conditions via deferred correction, Computational Methods in Applied Mathematics, vol. 23, no. 1, pp. 219–250, 2023. DOI: 10.1515/cmam-2021-0167.
[19] D. Hou, L. Ju, and Z. Qiao, A linear doubly stabilized Crank-Nicolson scheme for the Allen–Cahn equation with a general mobility, Advances in Applied Mathematics and Mechanics, vol. 16, no. 5, pp. 1009–1038, 2024.
[20] L. Reischmann and M. A. Peter, Multiscale modeling and simulation of a Cahn–Larché system with phase separation on the microscale, SIAM Journal on Applied Mathematics, vol. 80, no. 5, pp. 2170–2193, 2020. DOI: 10.1137/20M1321103.
[21] A. M. Turing, The Chemical Basis of Morphogenesis, Philosophical Transactions of the Royal Society of London. Series B, Biological Sciences, vol. 237, no. 641, pp. 37–72, 1952.
[22] J. Crank and P. Nicolson, A practical method for numerical evaluation of solutions of partial differential equations of the heat-conduction type, Proceedings of the Cambridge Philosophical Society, vol. 43, pp. 50–67, 1947.
[23] U. M. Ascher, S. J. Ruuth, and R. J. Spiteri, Implicit-Explicit Runge-Kutta Methods for Time-Dependent Partial Differential Equations, Applied Numerical Mathematics, vol. 25, no. 2-3, pp. 151–167, 1997.
[24] E. M. Constantinescu and A. Sandu, Extrapolated Implicit-Explicit Time Stepping, SIAM Journal on Scientific Computing, vol. 28, no. 2, pp. 411-432, 2007. DOI: 10.1137/05064607X.

Nermeen Shehab
Mathematics Department, Faculty of Science, Damietta University, New Damietta, Egypt
Email address: nermn_ahmd@du.edu.eg

Mohamed El-Shehawey
Mathematics Department, Faculty of Science, Damietta University, New Damietta, Egypt
Email address: el_shehawy@du.edu.eg

Ahmed M. A. El-Sayed
Faculty of Science, Alexandria University, Alexandria, Egypt
Email address: amasayed@alexu.edu.eg

Nasser Sweilam
Mathematics Department, Faculty of Science, Cairo University, Giza, Egypt
Email address: nsweilam@sci.cu.edu.eg