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Research Article

The Numerical Solution of Singularly Perturbed Nonlinear Partial Differential Equations in Three Space Variables: The Adaptive Explicit Inverse Preconditioning Approach

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Critical comments on the complexity of computational systems and the basic singularly perturbed (SP) concepts are given. A class of several complex SP nonlinear elliptic equations arising in various branches of science, technology, and engineering is presented. A classification of complex SP nonlinear PDEs with characteristic boundary value problems is described. A modified explicit preconditioned conjugate gradient method based on explicit inverse preconditioners is presented. The numerical solution of a characteristic 3D SP nonlinear parabolic model is analytically given and numerical results for several model problems are presented demonstrating both applicability and efficiency of the new computational methods.

1. Introduction

1.1. Complexity of Computational Systems. A wide spectrum of complex computational problems can be found in computer science and information management, as well as in different disciplinary fields, such as applied mathematics, engineering, business, finance, medicine, computational biology, social networks, transportation, telecommunications, education, government, and healthcare.

In recent times, complex systems of all types, like web-based systems, cloud infrastructures and big data centres, social networks, peer-to-peer, mobile and wireless systems, cyber-physical systems, the Internet of things, and real-time and embedded systems, have increasingly distributed, and dynamic system architectures providing high flexibility also increase the complexity of managing end-to-end application performance.

1.2. Singular Perturbation Problems. Singular perturbation (SP) problem in computer mathematics is a computational problem containing small parameters that cannot be approximated by setting the parameter values to zero; that is, the problem solution cannot be uniformly approximated by asymptotic expansions. The term singular perturbation was introduced in the 1940s by Wasow [1], and SP problems are generally characterized by dynamics operating on multiple scales.

Basic SP methods include the method of matched asymptotic expansions, the Poincaré–Lindsted method, the method of multiple scales and periodic averaging, and the WKB approximation for spatial problems [2–5]. Numerical techniques for solving nonlinear elliptic SP problems have been developed in several branches of science, technology, and engineering.

1.3. Topics of Various SP Problems. Topics of various problems are raised in several mathematical models in mathematical physics, optimization, and economic, where nonlinear PDEs of elliptic type arise almost in every scientific field. Solutions of such equations occur in diverse fields of mathematics, such as functional analysis, algebraic topology, differential geometry, variational calculus, and potential theory, while SP problems can occur in various areas of applied mathematics and engineering, i.e., fluid dynamics, fluid mechanics, quantum mechanics, magnetohydrodynamics, elasticity, chemical reactor theory, and reaction-diffusion processes. The topics of boundary-layer theory and approximation of solutions of various computational problems, where SP parameters (large or small) exist in complex solutions, and other critical problems require their analyses of asymptotic methods.

The asymptotic analysis for differential operators refers to operative perturbations over (very) narrow regions across dependent variables with very rapid chances, and the small parameters multiply the highest derivatives. These are usually referred very difficult for numerical solving, such as boundary layers in fluid mechanics, skin layers in electrical applications, shock layers in fluid and solid mechanics, transition points in quantum mechanics, Stokes lines, and surfaces. The terminology boundary layer has been introduced by Prandl [6], and since then, several 2D nonlinear SP problems remain unsolved [7].

During the last decades, several approximate methods for analysing nonlinear SP problems have been developed including the boundary-layer method, the method of averaging, the method of matched asymptotic expansion, and multiple scales, while a class of SP nonlinear boundary value problems for ODEs, the reaction-diffusion equations [8], the shock layer solution of nonlinear equations for SP problems, and problems of atmospheric physics [9] have been also developed.

The numerical solution of SP elliptic PDEs plays an important role in computational fluid dynamics for the simulation of flow problems [10, 11], but the derivation of computational discretization schemes appropriate for all types of linear and nonlinear SP elliptic equations is still an open problem. Note that the SP problems can be classified in numerical and asymptotic problems. Numerical analysis provides quantitative information about the given problem, while asymptotic analysis provides elements of quantitative behavior of classes of problems by giving semiquantitative information about any particular member of this class of problems.

In this research work, a modified version of the explicit adaptable preconditioned conjugate gradient method based on a new explicit inverse preconditioner is presented. The application of the new adaptable modified explicit preconditioned method, based on the new explicit preconditioner, leads to faster numerical solution of singular perturbed parabolic differential equations, especially in the case of three space variable problems. Note that proposed methods based on EPCG and inverse preconditioners by choosing the appropriate preconditioner lead to more accurate numerical solution methods than these with no preconditioner for solving distinct complex inverse problems. The usage of such powerful explicit inverse preconditioner, in the case that the original coefficient matrix of the given discretized partial differential equation is a nonsingular $(m \times n)$ nonsymmetric matrix of irregular structure, for solving complex computational problems, yields efficient solutions of 3D singular perturbation time-dependent differential equations.

2. Classification of SP Nonlinear PDEs

Many physical phenomena in science and engineering can be modelled as boundary value problems associated with various types of PDEs or systems of PDEs. During the solution of these models, the important qualities can be retained by omitting negligible quantities involving (very) small parameters. A class of several complex SP nonlinear elliptic equations arising in various branches of science, technology, and engineering has been recently presented [12]. For the application point of view such models include the following physical phenomena: nonlinear waves arising in gas dynamics, water waves, flood waves in rivers, transport of pollutants, chemical reactions, traffic flow, chromatography, and various biological and ecological systems.

These classes of applications contain nonlinear elliptic/parabolic equations with singular perturbation, such as the following characteristic equations:

(i) Reference [13] considered the problem arising in the study of reaction-diffusion systems with chemical or biological motivation:

$$\begin{aligned} -\varepsilon^2 \Delta u + u &= u^p, \quad u > 0 \text{ in } \Omega, \\ \theta\left(\frac{\partial u}{\partial \theta}\right) &= 0 \quad \text{on } \partial\Omega, \end{aligned} \tag{1}$$

where Ω is the bounded domain in R^n with smooth boundary $\partial\Omega$, ϑ denotes the unit outer normal at $\partial\Omega$, and $p \in (1, (n+2)/(n-2))$.

(ii) The standing waves of the nonlinear Schrodinger equation are considered by [14]

$$\begin{aligned} -\varepsilon^2 \Delta u + V(x)u = u^p, \quad u > 0 \text{ in } R^n,\ u > 0, \\ u \in W_{1,2}(R^n), \end{aligned} \tag{2}$$

where $p > 1$ is subcritical and V is the smooth bounded potential.

(iii) A basic model is the system, according to [15], which models the densities of a chemical activator U and an inhibitor V and is used to describe experiments of regeneration of hydra:

$$\begin{aligned} U_t &= d_1 \Delta U - U + \frac{U^p}{V^q} \quad \text{in } \Omega \times (0, +\infty), \\ V_t &= d_2 \Delta V - V + \frac{U^r}{V^s} \quad \text{in } \Omega \times (0, +\infty), \\ \frac{\partial U}{\partial \theta} &= \frac{\partial V}{\partial \theta}, \end{aligned} \tag{3}$$

where $d_1, d_2, p, q, r, s > 0$, with the constraints $0 < ((p-1)/q) < (r/(s+1))$.

(iv) Nerve impulse application concerns the following nonlinear elliptic singular perturbation equation:

$$\begin{aligned} -\varepsilon^2 \Delta u + f(u) + \varepsilon \gamma v &= 0 \quad \text{in } \Omega, \\ \Delta u + v - u &= 0 \quad \text{in } \Omega, \\ \partial_{\mathrm{v}} u &= \partial_{\mathrm{u}} v \quad \text{on } \partial\Omega, \end{aligned} \tag{4}$$

on the smooth bounded domain Ω. The perturbation parameter ε is positive and small.

Note that considerable research work in special topics of SP nonlinear differential equations has been recently presented [16–26].

Conclusively, it is stated that a wide variety of important problems in science and engineering have been formulated in terms of nonlinear elliptic SP PDEs, which model nonlinear waves, arising in gas dynamics, water waves, chemical reactions, transport of pollutants, flood waves in rivers, chromatography, traffic flow, and a wide range of biological and ecological systems.

2.1. SP Nonlinear Parabolic/Elliptic Differential Equations. SP parabolic first BV problems have been discussed by several researchers [27–29]. Various convection diffusion problems governed by second-order semilinear parabolic/elliptic equations with small parameters multiplying the second-order space derivatives subject to mixed types prescribed parabolic boundaries of the domains of the problems trying to determine how close the obtained approximate solution is to the actual solution of the problem [30, 31].

The differential equations

$$\frac{\partial u_i}{\partial t} = K_i \partial^2 u_i + O^* \left(t, x, u_1, u_2, \ldots, u_n\right), \quad i = 1, 2, \ldots, n, \tag{5}$$

when $K \geq 0$, which is sufficiently small, then the corresponding BV problem is a singular perturbation problem which arises in electrochemistry [32].

The area of SP is a field of increasing interest to applied mathematicians and computer mathematics scientists. During the last decades, considerable contributions on the topic and its applications have been made by several researchers [1, 32–41]. Note that considerable research work in special topics of SP nonlinear differential equations has been recently presented [16–21].

Conclusively, it is stated that a wide variety of important problems in science and engineering has been formulated in terms of nonlinear elliptic SP PDEs, which model nonlinear waves, arising in gas dynamics, water waves, chemical reactions, transport of pollutants, flood waves in rivers, chromatography, traffic flow, and a wide range of biological and ecological systems.

2.2. Solving Complex SP Nonlinear Problems: Recent Advances on Special Topics. Singular perturbation theory concerns the study of problem featuring parameters for which the solutions of problems at a limiting value of parameters are different in character from the limit of solutions of the general problem, i.e., the limit is singular. In contrast, for regular perturbation problems, the solutions of the general problem converge to solutions of the limit problem as the parameters approaches the limit values. Singular perturbation problems occur in a wide spectrum contexts, areas of applied mathematics, science and engineering, such as fluid mechanics (boundary-layer problems), elasticity (edge effort in shells), and quantum mechanics [19, 42–54].

Perturbation theory is a collection of methods for obtaining approximate solutions to problems involving small parameters ε. These methods are very powerful; thus sometimes it is actually advisable to introduce a parameter ε temporarily into a difficult problem having no small parameter, and then finally to set $\varepsilon = 1$ to recover the original problem. The approach of perturbation theory is to decompose a difficult problem into a (infinite) number of relatively easy ones. The perturbation theory is most useful when the first few steps reveal the important features of the solution and the remaining ones give small corrections. Perturbation solutions can be classified into two types. A basic feature of regular perturbation problems is that the exact solution for small but nonzero ε smoothly approaches the unperturbed solution as $\varepsilon \longrightarrow 0$. A singular perturbation problem is defined as the one whose solution for $\varepsilon = 0$ is fundamentally different in character from the "neighbouring" solutions obtained in the limit $\varepsilon \longrightarrow 0$ [53, 55–64].

Singular perturbation theory concerns the study of problems featuring parameters for which the solutions of problems at a limiting value of parameters are different in character from the limit of solutions of the general problem; that is, the limit is singular. In contrast, for regular perturbation problems, the solutions of the general problem converge to solutions of the limit problem as the parameters approach the limit values.

The computational singular perturbation (CSP) method [65] is a commonly used method for finding approximations of slow manifolds in systems of ordinary differential equations (ODEs) with multiple time scales. The validity of the CSP method was established for fast-slow systems with a small parameter [42, 44, 46, 52–54, 61, 66, 67].

3. Numerical Solution of a 3D SP Nonlinear Parabolic Model

Let us consider the general SP quadratically nonlinear elliptic Dirichlet problem:

$$\begin{aligned} &\varepsilon \Delta u = A(x,u)(\nabla u, \nabla u) + B(x,u)\nabla u + C(x,u), \quad x \in \Omega, \\ &u(x,\varepsilon) = f(x) \quad \text{for } x \text{ on } \Gamma, \end{aligned} \tag{6}$$

where Ω is an open and bounded set in Euclidean n-space E^n; Γ is the boundary of Ω; and A, C, a, f, and B are smooth functions, while the parameter ε is a very small, positive number [68].

Let us consider a class of singular perturbation (SP) nonlinear parabolic partial differential equation (PDE) in three space dimensions of the form:

$$\begin{gathered} \left(\frac{\partial u}{\partial t}\right) \varepsilon_{\mathrm{sp}} \Delta u(x, y, z, t) = e^n, \quad \varepsilon_{\mathrm{sp}} \longrightarrow 0_+, \\ (x, y, z) \in R \text{ and } t \geq 0, \end{gathered} \tag{7}$$

where Δ is the operator ($\Delta \equiv ((\partial/\partial x), (\partial/\partial y), (\partial/\partial z))$); $\varepsilon_{\mathrm{sp}}$ is the real SP parameter; c and β are the real parameters; and t is the time, subject to the boundary conditions

$$u(x, y, z, t) = a, \quad t > 0, \ (x, y, z) \in \partial R, \tag{8}$$

and the initial conditions

$$u(x, y, z, 0) = g(x, y, z), \quad 0 \le x, \ y, \ z \le \gamma. \tag{9}$$

The nonlinear PDE can be solved, after the FD/FE discretization by a linearized inner-outer iterative scheme, where the outer iteration is carried out by a Newton iteration of the form

$$\begin{aligned} &\left[\frac{h^2}{\varepsilon_s}\right]\left[\frac{1}{\Delta t} - e^{u(k)}\right]u_{i,j}^{(k+1)} - L_h u_{i,j}^{(k+1)} \\ &\quad = \left[\frac{h^2}{\varepsilon_s}\right]\left[\frac{e^{u(k)}}{\Delta t} + \left[1 - u^{(k)}\right]e^{u(k)}\right], \end{aligned} \tag{10}$$

where L_h is the discretized differential operator. The backwards difference process can be used for the discretization of time.

The resulting nonlinear system is

$$A_k u^{(k+1)} = s\left[u^{(k)}\right], \quad k > 0. \tag{11}$$

The inner iterative scheme can be performed by using an explicit preconditioned conjugate gradient method with termination criterion:

$$\left\|r_i\right\|_\infty < 10^{-4}, \tag{12}$$

while the outer iteration termination criterion was chosen as

$$\max_{j\in[1,n]}\left\{\frac{\left[u_j^{(k+1)} - u_j^{(k)}\right]}{\left[1 + u_j^{(k)}\right]}\right\} < 10^{-5}. \tag{13}$$

Note that m and p are the semibandwidths of the coefficient matrix; l_1 and l_2 are the width parameters in semibandwidths m and p, respectively; r_1 and r_2 are the fill-in parameters in semibandwidths m and p, respectively; and δl_i are the so-called "retention" parameters; that is, the number of diagonals retained in approximate inverse matrix [69]. For the numerical experimentation, the values of the fill-in parameters were chosen as $r_1 = r_2 = 2$ and the width parameters were chosen as $l_1 = l_2 = 3$.

4. Modified Explicit Preconditioned Conjugate Gradient Method

Let us assume that the coefficient matrix in Section 1.3 is in general a large nonsingular real unsymmetric matrix of semibandwiths m and p, respectively, retaining nonzero elements in widths l_1 and l_2 retaining r_1 and r_2 fill-in terms, respectively. The coefficient matrix A is considered to be a banded matrix of irregular structure. Let us also consider that there is a class of approximate inverses of A, with M the exact inverse of A [69].

Then, the following subclasses of approximate inverses, depending on the accuracy, storage, and computational work requirements, can be derived as it is shown in (14):

$$A^{-1} \equiv M \xrightarrow{\text{Subclass I}} M_{r_1=m-1,r_2=p-1}^{\delta l_1,\delta l_2} \xrightarrow{\text{Subclass II}} M^{S}{}_{r_1=m-1,r_2=p-1}^{\delta l_1,\delta l_2} \xrightarrow{\text{Subclass III}} M_{r_1,r_2}^{\delta l_1,\delta l_2} \xrightarrow{\text{Subclass IV}} M^{*}{}_{r_1,r_2}^{\delta l_1,\delta l_2} \equiv M^* \tag{14}$$

where $M^{S}{}_{r_1=m-1,r_2=p-1}^{\delta l_1,\delta l_2}$ of subclass I is a banded form of the exact inverse retaining δl_1 and δl_2 elements along each row and column, respectively, while its elements are equal to the corresponding elements of the exact inverse. The term $M^{S}{}_{r_1=m-1,r_2=p-1}^{\delta l_1,\delta l_2}$ of subclass II is a banded form of M, retaining only δl_1 and δl_2 elements along each row and column during the computational procedure of the approximate inverse, and under certain hypotheses, it can be considered as a *good approximation* of the original inverse, while the entries of the approximate inverse in subclass III have been retained after computing $M^* \, (r_1 < m - 1$ and $r_2 < p - 1)$ and are less accurate than the corresponding entries of $M^{*}{}_{r_1,r_2}^{\delta l_1,\delta l_2}$. Finally, in subclass IV, the elements of the approximate inverse can be computed [70–72].

The SP nonlinear parabolic system can be solved by using an inner-outer iterative scheme. In this section, a modified explicit preconditioned conjugate gradient method is presented.

4.1. Adaptive Preconditioned Conjugate Gradient Method Using the Explicit Approximate Preconditioner. The PCG method can solve the problem $\min\|b - AR^{-1}x\|$, where R is the sparse, nonsingular QR factor, while the preconditioned CGLS method can solve the following equations: $M = R^T R$, $R^{-T} A^T A R^{-1} \ u = R^{-T} A^T b$, and $u = Rx$. In order to compute efficiently the solution of the linear system $Ax = b$, a modified explicit preconditioned conjugate gradient (mEPCG) method is applied in the format of Algorithm 1.

This algorithm requires the additional work that is needed to solve the linear system

$$\varepsilon_P M^* \tilde{r}_n = r_n, \tag{15}$$

once per iteration. Therefore, the preconditioner ($\varepsilon_P \, M^*$) should be chosen such that the process can be done easily and efficiently.

The preconditioner ($\varepsilon_P \, M^*$) $= G$ that results in a minimal memory use. The storage requirement was the vectors r, x, y, and p and the upper triangular matrix G, in the data implementation. The convergence rate of preconditioned CG is independent of the order of equations, and the matrix vector products are orthogonal and independent. The preconditioned CG method in not self-correcting and the numerical errors accumulate every iteration. Therefore, to minimize the numerical errors in the PCG, double precision variables were used at the cost of memory usage. An explicit PCG method of second order can be alternatively used in conjunction with the explicit approximate inverse M_μ^* for solving complex computational problems with the appropriate selection of the iterative parameters [71].

Purpose: a modified PCG method is used for solving a given system of linear equations
Input: A is a symmetric and positive definite coefficient matrix, b is the right-hand side vector, tol is the predermined tolerance, x_0 is the initial guess, ε_P is a SP-inverse parameter, and M^* is the required inverse preconditioner
Output: x the solution vector.
Computational Procedure
Step 1: given x_0, ε_P SP-inverse parameter, inverse preconditioner M^*
Step 2: set $r_0 = A * x_0 - b$
Step 3: solve $\varepsilon_P M^* y_0 = r_0$, for y_0
Step 4: set $p_0 = -y_0, \quad k = 0$
Step 5: while $r_k \neq 0$
Step 6: compute a step length $a_k = (r_k^T * y_k)/(p_k^T A * p_k)$
Step 7: update the approximate solution $x_{k+1} = x_k + a_k * p_k$
Step 8: update the residual $r_{k+1} = r_k + a_k * A * p_k$
Step 9: solve $(\varepsilon_P M^*) \cdot y_{k+1} = r_{k+1}$
Step 10: compute a gradient correction factor $\beta_{k+1} = (r_{k+1}^T * y_{k+1})/(r_k^T * y_k)$
Step 11: set the new search direction $p_{k+1} = -y_{k+1} + \beta_{k+1} * p_k$
Step 12: $\kappa = \kappa + 1$
Step 13: end (while)

Algorithm 1: mEPCG $(A, b, \text{tol}, x_0, \varepsilon_P, M^*, x)$.

5. Numerical Results

Let us consider a characteristic singular perturbation (SP) nonlinear parabolic PDE in three space dimensions in a predetermined region. The FE discretization of this problem leads to the solution of a nonlinear system, where the coefficient matrix is a nonsingular, large sparse nonsymmetric $(n \times n)$ matrix of irregular structure [73]. In order to demonstrate both capabilities and efficiency of the proposed methods, a model problem has been selected and corresponding numerical results are indicatively presented.

Two hybrid inner-outer iterative methods have been considered, i.e., the Newton-mEPCG method, with inner iteration the modified explicit preconditioned conjugate gradient (mEPCG) method, and the Newton-EPBICG-STAB method, with inner iteration the explicit preconditioned biconjugate conjugate gradient (EPBICG-STAB) method.

The convergence behavior of Newton (outer iteration) and mEPCG/EPBICG-STAB (inner iteration) is shown in Tables 1–4 and Figures 1 and 2 for a model problem of n = 3375, $m = 26$, and $p = 226$, with several values of SP parameter ε_S, selected values of time step Δt, and several values of retention parameters δl.

The explicit preconditioned biconjugate conjugate gradient-STAB (EPBICG-STAB) method and variants have been presented in related research works [73, 74]. It should be noted that the explicit preconditioning methods and explicit approximate inverse combined with appropriate preconditioners can be applied in a wider application fields in applied and computer mathematics, while explicit approximate inverses can be combined with multigrid methods and other related hybrid computational techniques.

Table 1: The convergence behavior of Newton-mEPCG method for solving the given nonlinear problem (time step $\Delta t = 0.010$).

	Inner iterations (method mEPCG)			Δt	Outer iterations (method Newton)
ε_S	1	m	p		
1.00	49	42	34		6
0.10	98	96	81	0.010	16
0.01	333	369	342		93

Table 2: The convergence behavior of Newton-EPBICG-STAB method for solving the given nonlinear problem (time step $\Delta t = 0.010$).

	Inner iterations (method EPBICG-STAB)			Δt	Outer iterations (method Newton)
ε_S	1	m	p		
1.00	28	28	22		6
0.10	64	63	52	0.01	16
0.01	243	252	234		93

Table 3: The convergence behavior of Newton–mEPCG method for solving the given nonlinear problem (time step $\Delta t = 0.005$).

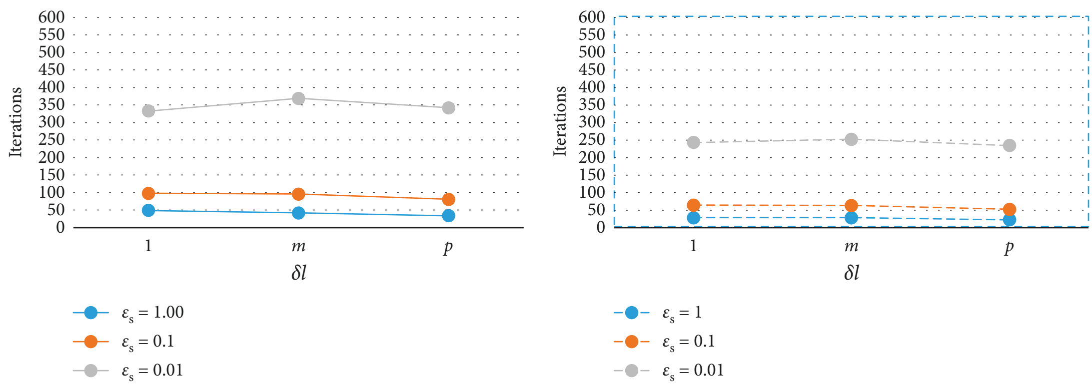
	Inner iterations (method mEPCG)			Δt	Outer iterations (method Newton)
ε_S	1	m	p		
1.00	57	50	42		7
0.10	129	131	114	0.005	25
0.01	527	594	557		165

6. Conclusions

Basic elements of complexity and singularly perturbed concepts have been discussed. A classification of complex SP nonlinear elliptic equations arising in various branches of science and engineering in the form of a two-decade survey has been presented.

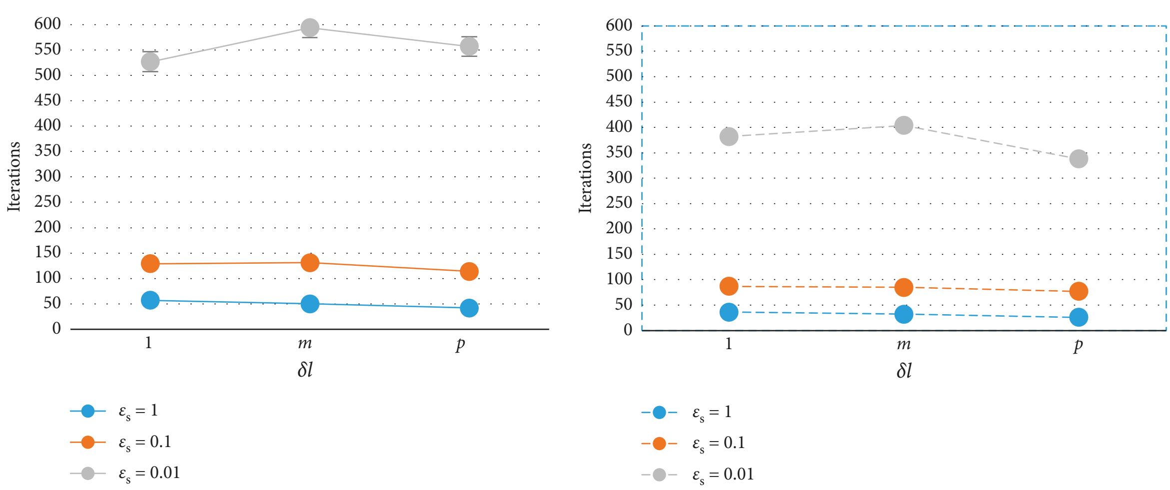
Table 4: The convergence behavior of Newton-EPBICG-STAB method for solving the given nonlinear problem (time step $\Delta t = 0.005$).

ε_S	Inner iterations (method EPBICG-STAB) 1	m	p	Δt	Outer iterations (method Newton)
1.00	36	32	26		7
0.10	87	85	77	0.005	25
0.01	382	404	338		165



(a) (b)

Figure 1: Inner iterations (methods mEPCG (a) and EPBICG-STAB (b)) of the hybrid schemes Newton-mEPCG and Newton-EPBICG-STAB with $\Delta t = 0.01$.



(a) (b)

Figure 2: Inner iterations (methods mEPCG (a) and EPBICG-STAB (b)) of the hybrid schemes Newton-mEPCG and Newton-EPBICG-STAB with $\Delta t = 0.005$.

A modified explicit preconditioned conjugate gradient method based on explicit inverse preconditioners is introduced for solving complex nonlinear parabolic problems. The numerical solution of a characteristic SP nonlinear initial/boundary value is presented, and numerical results demonstrating both applicability and effectiveness of the derived new methods are given. Future research work is planned towards the implementation of the new computational methods in parallel computer environments.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The author declares that there are no conflicts of interest regarding the publication of this paper.

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