Applied Mathematics and Computation 254 (2015) 266–276

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

A multigrid preconditioned numerical scheme for a reaction–diffusion system

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ARTICLE INFO

Keywords:
Reaction–diffusion system
Gray Scot model
Predator prey model
Finite difference scheme
Multigrid solver

ABSTRACT

Reaction diffusion operators have been used to model many engineering and biological systems. In this study we consider a reaction diffusion system modeling various engineering and life science problems. There are many algorithms to approximate such mathematical models. Most of the algorithms are conditionally stable and convergent. For a big time step size a Krylov subspace type solver for such models converges slowly or oscillates because of the presence of the diffusion term. Here we study a multigrid preconditioned generalized minimal residual method (GMRES) for such a model. We start with a five point scheme for the spatial integration and a method of lines for the temporal integration of the system of PDEs. Then we implement a multigrid iterative algorithm for the full discrete model, and show some numerical results to demonstrate the dominance of the solver. We analyze the convergence rate of such a multigrid iterative preconditioning algorithm. Reaction diffusion systems arise in many mathematical models and thus this study has many applicabilities.

1. Introduction

Reaction diffusion systems are a class of parabolic partial differential equations (PDEs). There are many problems from physics, chemistry, engineering, biology as well as ecology that can be expressed by using parabolic system of PDEs [5,4,6,11–13,9,18,8,16,7,10]. Considering a bounded spatial domain Ω and a finite time interval $[0,T]$, in this work, we study numerical solutions of the following 2-component reaction–diffusion systems [4,6,13] over $\Omega \times (0,T)$

$$\begin{aligned} \frac{\partial u}{\partial t} &= \delta_1 \Delta u + f(u,v), \\ \frac{\partial v}{\partial t} &= \delta_2 \Delta v + g(u,v), \end{aligned} \tag{1}$$

where $\Delta w = \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2}$ with

$$u(x,y,0) = u_0(x,y), \quad v(x,y,0) = v_0(x,y), \quad (x,y) \in \Omega \tag{2}$$

and

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http://dx.doi.org/10.1016/j.amc.2014.12.062
0096-3003/

$$\frac{\partial u}{\partial \nu} = \frac{\partial v}{\partial \nu} = 0, \text{ on } \partial\Omega \times (0,T), \tag{3}$$

ν denotes the outward normal to $\partial\Omega$. The nonlinearities $f(u,v)$ and $g(u,v)$ are chosen in order to fit the real world problem considered to model. For example the following two set of nonlinearities are considered to model predator–prey interactions [4,11]

1. $f(u,v) = u(1-u) - \frac{uv}{u+\alpha}$ and $g(u,v) = \frac{\beta uv}{u+\alpha} - \gamma v$,
2. $f(u,v) = u(1-u) - v(1-e^{-\gamma u})$ and $g(u,v) = \beta v(\alpha - 1 - \alpha e^{\gamma u})$;

whereas the set of nonlinearities

3. $f(u,v) = F(1-u) - uv^2$ and $g(u,v) = uv^2 - (F+k)v$

is considered to model an engineering problem, well known as the Grey Scot model [6,13].

A detailed study about these nonlinearities and stability issues of such system of resulting ODEs (dropping the diffusion terms) can be founded in [12,13]. They discuss the applicability and suitability of these nonlinearities modeling various engineering, biological, ecological and chemical reality. Authors in both communications discuss the stability conditions and bifurcation issues of solutions. A brief discussion about the predator–prey interactions model and the Grey Scot model is available in the appendix.

These models are complicated to analyze. Because of the nonlinearity it is almost impossible to have an exact solution. So scientists rely on an approximate solution to understand the dynamics of the physical/chemical/biological reality modeled. Many finite difference schemes and finite element schemes for space integration followed by some time stepping schemes (method of lines) for time integration have been popularly using to approximate solutions [4,13]. These schemes produce a huge system of equations, and thus an inversion is needed to get approximate solutions.

Medvinsky et. al. presents various theoretical and numerical issues of the model problem (1) in their noble work in [11]. They present some pattern formations of solutions numerically for different choices of initial conditions and parameter values. They have an extensive list of references what one can use for further study about these type of models with various engineering and scientific applications. But no discussion about an efficient linear system solver for this model is available here.

Recently Chang et. al. [2] discuss a numerical parameter continuation method for a nonlinear reaction diffusion system to analyze the bifurcations and chaos. They start the study by discussing some sophisticated linear solvers (GMRES, BiCGSTAB, MG). Then they discuss a numerical path continuing method to solve/approximate a parameter dependent reaction diffusion system (similar to arc length continuation methods to detect stability/bifurcations). They discuss the difficulties of handling their problem when solutions reach to singularity or close to singularity. Then propose to use multigrid method to solve the linear system. In each relaxation step inside the MG iteration they employ GMRES/Bi-CGSTAB (with/without preconditioning) to improve the solutions. Here the operator used to for preconditioning the GMRES is missing as well as an analysis of the convergence factor of the MG method is missing.

There are many articles that use conjugate gradient algorithm/generalized mean residual algorithm to approximate the solutions of the resulting system of equations [14,4,15]. Convergence is an issue of using these type of iterative solvers. Authors in [4,5] consider the system of PDEs (1) with nonlinearities of type 1 and 2. They discuss some basic mathematical properties about the systems before they attempt numerical solutions of the model. They approximate the PDEs using a finite difference scheme [4] and a finite element scheme [5] for the spatial integration, and then a method of lines for the time integration. For the resulting system of equations they employ the GMRES algorithm. The authors mainly focus on discussing evolution of solutions.

From our computational experiences as well as following various articles [1,3,17,15] we notice that because of the presence of the diffusion operator krylov subspace type solvers converge slowly for a large choice of time stepping. That is to say that they need many iterations to converge. As a result the schemes become computationally expensive. But a suitable choice of a preconditioner can improve the situation [3]. In this study we propose a multigrid preconditioned GMRES iterative solver for the nonlinear system of PDEs (1) and analyze the asymptotic convergence rate of the iterative solver.

To be specific we study the efficiency of a multigrid accelerated generalized minimal residual method (GMRES) for the system of PDEs (1). To that end we start with an implicit one step scheme for the time integration and a 5 point scheme for the spatial approximation for the system. Then we employ the standard Newton's algorithm for the resulting nonlinear system of equations. In each inner step of the Newton's nonlinear solver we employ a multigrid preconditioned GMRES iterative algorithm for the system of linear equations and investigate the efficiency of the algorithm. Here we split the discrete version of (1) into two nonlinear system of equations and apply a multigrid accelerated GMRES algorithm for the resulting system which is simple in terms of implementations and storage costs. In this way the convergence analysis of the multigrid algorithm for the resulting system is also less complicated than that of the full discrete nonlinear system of PDEs (1). We analyze the rate of convergence of the multigrid iterative algorithm as well. A noticeable improvement in terms of convergence rate of the GMRES solver has been achieved by employing a two grid preconditioner. Here we notice that a multigrid