Applied Mathematics and Computation 231 (2014) 445–462

Contents lists available at ScienceDirect

Applied Mathematics and Computation

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

A finite volume method with linearisation in time for the solution of advection–reaction–diffusion systems

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ARTICLE INFO

Keywords:
Nonlinear
Reaction
Advection
Diffusion
Shock
Chemotaxis
Finite volume method

ABSTRACT

The numerical solution in one space dimension of advection–reaction–diffusion systems with nonlinear source terms may invoke a high computational cost when the presently available methods are used. Numerous examples of finite volume schemes with high order spatial discretisations together with various techniques for the approximation of the advection term can be found in the literature.

Almost all such techniques result in a nonlinear system of equations as a consequence of the finite volume discretisation especially when there are nonlinear source terms in the associated partial differential equation models.

This work introduces a new technique that avoids having such nonlinear systems of equations generated by the spatial discretisation process when nonlinear source terms in the model equations can be expanded in positive powers of the dependent function of interest.

The basis of this method is a new linearisation technique for the temporal integration of the nonlinear source terms as a supplementation of a more typical finite volume method. The resulting linear system of equations is shown to be both accurate and significantly faster than methods that necessitate the use of solvers for nonlinear system of equations.

1. Introduction

The use of advection–reaction–diffusion (ARD) equations for modelling biological processes can provide insight and perspective into the development of complex yet robust behaviour in living systems, that otherwise is difficult to achieve by direct or indirect observation of a living system. As a result, there exists now a substantial and increasing body of literature dealing with mathematical models of phenomena as diverse as tumour growth and invasion [1], the movement of cells in tissues [2] and pattern formation [3].

Usually the transport component of such models are dominantly diffusive or dominantly advective but there is a developing interest in problems where the contribution of both processes is important as indeed are the magnitudes of the reaction terms [4]. Although some traction in determining the behaviour of such systems may be gained by examining them at diminishing limits of diffusion or advection, the numerical solution of the full system can prove problematic. Such is the case for the mathematical models of embryologic development [5] where the system smoothly makes the transition from being dominantly parabolic, exhibiting smooth-fronted travelling waves, to dominantly hyperbolic with shock-fronted travelling

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0096-3003/$ - see front matter
http://dx.doi.org/10.1016/j.amc.2013.12.179

waves. Typically the methods adopted to reliably capture the travelling wavefronts in such models employ flux-limiting or gradient averaging techniques at the front [4].

Here we introduce a new method for numerically solving such ARD systems in one space dimension, based on the usual finite volume paradigm [6] with a third order upwinding scheme [7] for the calculations of the advection term in space and by employing a very effective integral approximation technique in time for chosen nonlinear reaction terms. This temporal integration approximation has been used in finite element and finite difference methods for solving partial differential equations where source term linearisation is required, see for example [8,9]. We find that the use of this linearisation technique in a finite volume method for solving the problems of our interest has been very effective in terms of computational cost for the simulations. We illustrate how the numerical scheme is implemented for a class of multi-species partial differential equation models where the diffusion component of each balance equation is taken to be Fickian and the advective velocity depends upon the gradient of another species. Such models are typically used in the description of chemotactic phenomena where cellular invasion is directed by a diffusive attractant [4,5]. We also demonstrate the effectiveness of the method described here by resolving a number of recent example models within this domain of advection–reaction–diffusion systems.

These models usually conform to the following description of two (or more) interacting species $u(x,t)$ and $c(x,t)$ say, both of which disperse by a process modelled as Fickian diffusion. Additionally species $u(x,t)$, usually taken to be a population density of some cellular species in time t at position x, is being advectively transported with a velocity determined by the gradient of another species $c(x,t)$. As a generic example of such systems we will take the following equations to hold for $0 < x < L < \infty$ and $t > 0$;

$$\frac{\partial u}{\partial t} = D_u \frac{\partial^2 u}{\partial x^2} - \frac{\partial}{\partial x}\left(u\chi(c)\frac{\partial c}{\partial x}\right) + f(u,c) \tag{1}$$

$$\frac{\partial c}{\partial t} = D_c \frac{\partial^2 c}{\partial x^2} + h(u,c) \tag{2}$$

where $f(u,c)$ and $h(u,c)$ describe the reaction between the species, and D_u and D_c are diffusion coefficients. The function $\chi(c)$ describing the sensitivity of the cells to the chemotactic signal is variously taken to be a constant or a nonlinear function of c, for example $\chi(c) = \kappa,\ \chi(c) = 1/(1+\kappa c)$ or $\chi(c) = \kappa c^2 - \kappa c + 1$ where κ is a constant [10]. Initial and boundary conditions may be generally represented as appropriate.

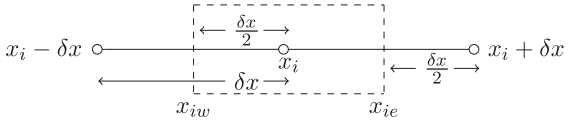
Although we are considering here only one dimensional systems involving 2 or 3 species, the methods described naturally extend to higher dimensional problems with more species.

2. Discretisation of equations using finite volume method

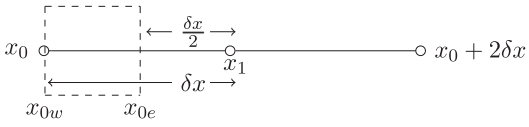
The model equations are discretised using the vertex centered control volume method with a uniform mesh. The nodes, $x_i = i\delta x,\ i = 0,1,2,3,\ldots,N$, are chosen along the x-axis between $x = x_0 = 0$ and $x = x_N = L$; where $N\delta x = L$. Control volumes are constructed around the interior nodes with control volume faces at $x_{iw} = x_i - \frac{\delta x}{2}$ and $x_{ie} = x_i + \frac{\delta x}{2}$ for $i = 1,2,3,\ldots,N-1$ as shown in Fig. 1(a). At the ends of the domain $[0, \frac{\delta x}{2}]$ and $[L - \frac{\delta x}{2}, L]$, see Fig. 1(b), are considered as the boundary control volumes.

Integration of Eq. (1) over the control volume $[x_{iw}, x_{ie}] = \left[x_i - \frac{\delta x}{2}, x_i + \frac{\delta x}{2}\right]$ w.r.t. x gives the following equation:

$$\frac{\partial}{\partial t}\left(\int_{x_{iw}}^{x_{ie}} u\,dx\right) = D_u\left[\frac{\partial u}{\partial x}\right]_{x_{iw}}^{x_{ie}} - \left[u\chi(c)\frac{\partial c}{\partial x}\right]_{x_{iw}}^{x_{ie}} + \int_{x_{iw}}^{x_{ie}} f(u,c)\,dx$$



(a) An interior control volume.



(b) A boundary control volume.

Fig. 1. Interior and boundary control volumes.