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ScienceDirect
Journal of Computational Physics 225 (2007) 6–12
JOURNAL OF COMPUTATIONAL PHYSICS
www.elsevier.com/locate/jcp

Short Note

Nonmonotone chemotactic invasion: High-resolution simulations, phase plane analysis and new benchmark problems

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Received 7 December 2006; received in revised form 20 March 2007; accepted 22 March 2007
Available online 31 March 2007

Keywords: Hyperbolic conservation law; Chemotaxis; Invasion; High-resolution methods; Shocks

1. Introduction

Verifying and validating the performance of a computational simulation is a challenging problem of interest in all applied sciences [12,13]. Measuring the performance of a numerical algorithm against standard benchmark test cases is often the first step in assessing algorithm performance. These test cases are used repeatedly over long periods of time as algorithms are devised and improved. In addition, new benchmark test cases are continually developed [9]. Effective benchmarks are characterized by having either a complete or an approximate analytical solution against which the numerical results can be quantitatively compared [1,5]. It is also possible, although less common, to use carefully collected laboratory data to benchmark a numerical code [18,22].

To identify an effective benchmark test case, a balance must be found between two opposing requirements: the benchmark ought to be sufficiently complex to rigorously challenge a numerical algorithm, and it should also be amenable to analysis.

Certain problems have become synonymous with algorithm development in various disciplines. Particular problems from fluid mechanics, for example, are associated with long-celebrated benchmarks. Algorithms designed to solve steady incompressible Navier–Stokes flows are often tested with lid-driven cavity flow problems and Burggraf's solution [1,3]. Algorithms designed to solve convectively-driven flow in porous media are usually benchmarked with Henry's solution for salt water intrusion [5,19]. Many other examples of popular benchmark test cases can be found in the literature.

Constructing numerical algorithms to accurately approximate the solution of hyperbolic conservation laws (HCL) is of wide interest and challenging. Typically HCL algorithms are tested with a suite of benchmark problems starting with single species linear advection [2,3,6,10]. Linear advection has the advantage of being conceptually simple, analytically tractable and clearly identifies susceptibility to numerical diffusion and

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0021-9991/$ - see front matter
doi:10.1016/j.jcp.2007.03.016

artificial oscillation. Beyond single species linear advection, algorithms are often benchmarked with Burger's equation. This problem retains the simplicity of a single species HCL with the complexity of introducing a nonlinear flux which tests an algorithm's ability to predict shock formation. Perhaps the most common benchmark for HCL algorithms is Sod's shock tube problem [21]. This is a rigorous benchmark requiring the solution of three coupled nonlinear equations. Sod's shock tube problem is used to test whether a code can predict solutions with multiple discontinuities. Variants of Sod's problem have been used for code development in numerous applications including dam break phenomena [23], star formation [17] and the dynamics of volcanic ash plumes [14].

Although various other HCL benchmarks are used for algorithm development, such as traffic flow problems, acoustic dynamics and the Buckley–Leverett equation [2,3,6,10], there does not appear to be any particular problem more complex than the shock tube problem that has become a clear standard choice for benchmarking. We propose a new test case which has arisen in computational biology relevant to chemotactic cell invasion [15,20]. The invasion problem involves nonlinearities and coupling in both the flux and source terms. These features make the numerical solution of the invasion problem more challenging than the shock tube problem. However, at the same time, many properties of traveling wave solutions to the invasion problem can be deduced exactly with nonstandard phase plane analysis. The invasion problem is sufficiently rigorous that it tests an algorithm's ability to approximate solutions with multiple discontinuities and complicated nonmonotone profiles.

A major historical difficulty in developing numerical algorithms for HCLs is the formation of artificial numerical oscillations. These oscillations often appear close behind a shock [10,21]. In this work we present an unusual test case where the true analytical solution is nonmonotone with an oscillatory region appearing just behind a shock. Therefore the correct solution has certain properties which are not shared by standard benchmark test cases.

We will briefly present the invasion model, describe the analysis, specify certain test cases and quantitatively compare numerical and analytical results. The details of a suite of solutions are tabulated for benchmarking purposes.

2. Chemotactic invasion model

Conservation of mass for chemotactic migration of cells with density n and chemoattractant concentration g in one spatial dimension gives

$$\frac{\partial n}{\partial t} = -\frac{\partial}{\partial x}\left(\chi(g)n\frac{\partial g}{\partial x}\right) + f(n), \quad \frac{\partial g}{\partial t} = h(g,n). \tag{1}$$

Here x is the spatial coordinate, t is time and $\chi(g)$ is the chemotactic sensitivity function. In these scaled equations we specify the source term for n as a logistic proliferation term $f(n) = n(1-n)$. The source term for g incorporates zeroth order production, linear decay and a nonlinear uptake term as given by $h(g,n) = \beta(1-g) - \gamma ng$. This system is strictly hyperbolic and details of the scaling used to nondimensionalize Eq. (1) are given elsewhere [20].

Most applications of hyperbolic invasion models make use of a constant $\chi(g)$ [15,20]. For initial conditions $n(x,0)$ with compact support, the traveling wave solutions are monotonically decreasing and shock-fronted. Recent theoretical work has demonstrated the existence of a wide range of traveling wave solutions with complex nonmonotone shapes and multiple discontinuities [8]. These solutions are obtained by using different $\chi(g)$ functions. The intricate detail of these solutions means that they are ideal for benchmarking since several features of the solution, such as the speed of invasion, length and position of discontinuities and the location of turning points in the solution can be used for algorithm benchmarking.

3. Phase plane analysis

Introducing the traveling wave coordinate for right-moving waves, $z = x - ct$ where $c > 0$ is the dimensionless wave speed, the conservation system can be written as a system of first order odes on $-\infty < z < \infty$: