Holistic finite differences accurately model the dynamics of the Kuramoto-Sivashinsky equation

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Abstract

We analyse the nonlinear Kuramoto-Sivashinsky equation to develop an accurate finite difference approximation to its dynamics. The analysis is based upon centre manifold theory so we are assured that

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the finite difference model accurately models the dynamics and may be constructed systematically. The theory is applied after dividing the physical domain into small elements by introducing insulating internal boundaries which are later removed. The Kuramoto-Sivashinsky equation is used as an example to show how holistic finite differences may be applied to fourth order, nonlinear, spatio-temporal dynamical systems. This novel centre manifold approach is holistic in the sense that it treats the dynamical equations as a whole, not just as the sum of separate terms.

Contents

1 Introduction

We continue exploring the new approach to finite difference approximation introduced by Roberts [10] by approximating the dynamics of solutions to the Kuramoto-Sivashinsky equation [4, 3, 5]. In some non-dimensional form we take the following partial differential equation (PDE) to govern the evolution of $u(x,t)$:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + R\frac{\partial^2 u}{\partial x^2} + \frac{\partial^4 u}{\partial x^4} = 0\,. \tag{1}$$

This model equation includes the mechanisms of linear growth u_{xx} controlled by the parameter R, high-order dissipation, u_{xxxx}, and nonlinear advection/steepening, uu_x. Consider implementing the method of lines by discretising in x and integrating in time as a set of ordinary differential equations. A finite difference approximation to (1) on a regular grid in x is straightforward, say $x_j = jh$ for some grid spacing h. For example, the linear term

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{j+1} - 2u_j + u_{j-1}}{h^2} + \mathcal{O}\left(h^2\right)\,.$$

However, there are differing valid alternatives for the nonlinear term uu_x: two possibilities are

$$u\frac{\partial u}{\partial x} = \frac{u_j(u_{j+1} - u_{j-1})}{2h} + \mathcal{O}\left(h^2\right) \tag{2}$$

$$\text{or} \quad u\frac{\partial u}{\partial x} = \frac{u_{j+1}^2 - u_{j-1}^2}{4h} + \mathcal{O}\left(h^2\right)\,. \tag{3}$$

Which is better? The answer depends upon how the discretisation of the nonlinearity interacts with the dynamics of other terms. The conventional approach of considering the discretisation of each term separately does not tell us. Instead, in order to find the best discretisation we consider the influence of all terms in the equation in a holistic approach.

As introduced in [10] and discussed in §2, centre manifold theory [1, 8, e.g.] has appropriate characteristics to do this. It addresses the evolution of a dynamical system in a neighbourhood of a marginally stable fixed point; based upon the linear dynamics the theory guarantees that an accurate low-dimensional description of the nonlinear dynamics may be deduced. For example the analysis herein supports the approximation (2) but with higher-order and nonlinear corrections. The analysis of the Kuramoto-Sivashinsky equation (1) in § 3 favours the discretisation

$$\begin{aligned}\frac{du_j}{dt} &+ \left[\frac{u_j(-u_{j+2}+9u_{j+1}-9u_{j-1}+u_{j-2})}{16h}\right.\\ &\left.+\left(\frac{u_{j+1}^2-u_{j-1}^2}{16h}\right)-\left(\frac{u_{j+2}u_{j+1}-u_{j-2}u_{j-1}}{48h}\right)\right]\\ &+R\left(\frac{-u_{j+2}+16u_{j+1}-30u_j+16u_{j-1}-u_{j-2}}{12h^2}\right)\\ &+\frac{u_{j+2}-4u_{j+1}+6u_j-4u_{j-1}+u_{j-2}}{h^4}=0\,, \end{aligned} \tag{4}$$

as a low-order approximation. Provided the initial conditions are not too extreme, centre manifold theory assures us that such a discretisation models

the dynamics of (1) to errors $\mathcal{O}(\|u\|^3, h^2)$. Such accuracy on a relatively coarse grid is extremely useful for such stiff PDEs. Further, because the centre manifold is composed of actual solutions to the dynamical system, we are assured that equation (4) models the whole of the Kuramoto-Sivashinsky equation, *independent* of its algebraic form.

The discretisation (4) is a low-order approximation, centre manifold theory also provides systematic corrections. Analysis to higher orders in the nonlinearity, discussed in § 3, shows higher order corrections to the discretisation of the nonlinear terms. The specific finite difference models presented here were derived by a computer algebra program. Computer algebra is an effective tool because of the systematic nature of centre manifold theory [9].

In this preliminary exploration of the approximation of the Kuramoto-Sivashinsky equation (1) we only consider an infinite domain or strictly periodic solutions in finite domains. Then all elements of the discretisation are identical by symmetry and the analysis of all elements is simultaneous. However, if physical boundaries to the domain of the PDE are present, then those elements near a physical boundary will need special treatment. Further research is needed on this and other issues.

2 Centre manifold theory underpins the fidelity

Here we describe in detail one way to place the discretisation of the Kuramoto-Sivashinsky equation (1) within the purview of centre manifold theory.

The discretisation is established via an equi-spaced grid of collocation points, $x_j = jh$ say, for some small spacing h. Here we scale the Kuramoto-Sivashinsky to the scale of the grid spacing h. Thus our view of the dynamics shrinks with h. This is different to the analysis in [10] and allows the linear dynamics to be dominated by simply the highest order spatial derivative term. We work on the scale of the grid by transforming (1) to the following space and time scales: $\xi = x/h$ (so that for example $\xi_j = j$) and $\tau = t/h^4$, giving

$$\frac{\partial u}{\partial \tau} + h^3 u \frac{\partial u}{\partial \xi} + h^2 R \frac{\partial^2 u}{\partial \xi^2} + \frac{\partial^4 u}{\partial \xi^4} = 0\,. \tag{5}$$

Then the crucial step: at midpoints $\xi_{j+1/2} = (\xi_j + \xi_{j+1})/2$ artificial boundaries are introduced:

$$\begin{bmatrix} \frac{\partial u^+}{\partial \xi} - \frac{\partial u^-}{\partial \xi} \\ \frac{\partial^3 u^+}{\partial \xi^3} - \frac{\partial^3 u^-}{\partial \xi^3} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tag{6}$$

$$\left(\frac{1-\gamma}{2}\right) \begin{bmatrix} \frac{\partial u^+}{\partial \xi} + \frac{\partial u^-}{\partial \xi} \\ \frac{\partial^3 u^+}{\partial \xi^3} + \frac{\partial^3 u^-}{\partial \xi^3} \end{bmatrix} = \gamma \mathcal{A} \begin{bmatrix} u^+ - u^- \\ \frac{\partial^2 u^+}{\partial \xi^2} - \frac{\partial^2 u^-}{\partial \xi^2} \end{bmatrix}, \tag{7}$$

where u^+ is just to the right of a midpoint and u^- to the left. These boundaries divide the domain into a set of elements, the jth element centred upon ξ_j and of width $\Delta\xi = 1$. When $\gamma = 0$ the right hand side of (7) disappears, thus the elements are effectively insulated from each other and so the solution is particularly simple, namely u is constant in each element. We use this simple class of solutions as a basis for analysing the $\gamma \neq 0$ case when the elements are coupled together. We are particularly interested in the approximation at $\gamma = 1$ when the grid scaled Kuramoto-Sivashinsky PDE (5) is effectively restored over the whole domain because (6–7) then ensure sufficient continuity between adjacent elements. The introduction of the near identity operator

$$\mathcal{A} = 1 + \frac{\partial_\xi^2}{12} - \frac{\partial_\xi^4}{720} + \frac{\partial_\xi^6}{30240} + \cdots = \frac{\partial_\xi}{2} \coth\left(\frac{\partial_\xi}{2}\right) , \tag{8}$$

ensures that high-order approximations to linear terms are obtained exactly as discussed in [10, §4]: it is remarkable that the exactly equivalent operator works for both Burgers' equation and the Kuramoto-Sivashinsky equation.

The following application of centre manifold theory to rigorously develop the above ideas is based upon a linear picture of the dynamics. Adjoin the dynamically trivial equations

$$\frac{\partial\gamma}{\partial\tau} = \frac{\partial h}{\partial\tau} = 0 , \tag{9}$$

and consider the dynamics in the extended state space $(u(\xi), \gamma, h)$. This is a standard trick used to unfold bifurcations [1, §1.5] or to justify long-wave approximations [6]. Within each element $u = \gamma = 0$ is a fixed point.

Linearized about each fixed point, that is to an error $\mathcal{O}\left(\|u\|^2+\gamma^2+h^2\right)$, the PDE is

$$\frac{\partial u}{\partial \tau}=\frac{\partial^4 u}{\partial \xi^4}\,, \quad \text{s.t.} \quad \left.\frac{\partial u}{\partial \xi}\right|_{\xi=\pm 1/2}=\left.\frac{\partial^3 u}{\partial \xi^3}\right|_{\xi=\pm 1/2}=0\,,$$

namely the hyperdiffusion equation with essentially insulating boundary conditions. There are thus linear eigenmodes associated with each element:

$$\gamma=0\,, \quad u\propto \begin{cases} e^{\lambda_n \tau}\cos[n\pi(\xi-\xi_{j-1/2})]\,, & \xi_{j-1/2}<\xi<\xi_{j+1/2}\,, \\ 0\,, & \text{otherwise}\,, \end{cases} \tag{10}$$

for $n=0,1,\ldots$, where the decay rate of each mode is $\lambda_n=-n^4\pi^4$; together with the trivial modes $\gamma=$ const, $h=$ const and $u=0$. In a domain with m elements, evidentally all eigenvalues are negative, $-\pi^4$ or less, except for $m+2$ zero eigenvalues: 1 associated with each of the m elements and 2 from the trivial (9). Thus, provided the nonlinear terms in (5) are sufficiently well behaved, the existence theorem ([2, p281] or [11, p96]) guarantees that a $m+2$ dimensional centre manifold $\mathcal{M}$ exists for (5–9). The centre manifold $\mathcal{M}$ is parameterized by γ, h and a measure of u in each element, say u_j: using $\boldsymbol{u}$ to denote the collection of such parameters, $\mathcal{M}$ is written as

$$u(\xi,\tau)=v(\xi;\boldsymbol{u},\gamma,h)\,. \tag{11}$$

In this the analysis has a very similar appearance to that of finite elements. The theorem also asserts that on the centre manifold the parameters u_j evolve deterministically

$$\dot{u}_j=g_j(\boldsymbol{u},\gamma,h)\,, \tag{12}$$

where $\dot{u}_j$ denotes $du_j/d\tau$, and g_j is the restriction of (5–9) to $\mathcal{M}$. In this approach the parameters of the description of the centre manifold may be anything that sensibly measures the size of u in each element—we simply choose the value of u at the grid points, $u_j(\tau) = u(\xi_j, \tau)$. This provides the necessary amplitude conditions, namely that $u_j = v(\xi_j; \boldsymbol{u}, \gamma, h)$. The above application of the theorem establishes that in principle we may find the dynamics (12) of the interacting elements of the discretisation. A low order approximation written in unscaled variables is given in (4).

The next outstanding question to answer is: how can we be sure that such a description of the interacting elements does actually *model* the dynamics of the original system (5–9)? Here, the relevance theorem of centre manifolds, [2, p282] or [11, p128], guarantees that all solutions of (5–9) which remain in the neighbourhood of the origin in $(u(\xi), \gamma, h)$ space are exponentially quickly attracted to a solution of the m finite difference equations (12). For practical purposes the rate of attraction is estimated by the leading negative eigenvalue, here $-\pi^4$. Centre manifold theory also guarantees that the stability near the origin is the same in both the model and the original. Thus the finite difference model will be stable if the original dynamics are stable. After exponentially quick transients have died out, the finite difference equation (12) on the centre manifold accurately models the complete system (5–9).

The last piece of theoretical support tells us how to approximate the shape of the centre manifold and the evolution thereon. Approximation theorems such as that by Carr & Muncaster [2, p283] assure us that upon substituting

the ansatz (11–12) into the original (5–9) and solving to some order of error in $\|u\|$, γ and h, then $\mathcal{M}$ and the evolution thereon will be approximated to the same order. The catch with this application is that we need to evaluate the approximations at $\gamma = 1$ because it is only then that the artificial internal boundaries are removed. In some applications of such an artificial homotopy good convergence in the parameter γ [7] has been found. Thus although the order of error estimates do provide assurance, the actual error due to the evaluation at $\gamma = 1$ should be also assessed otherwise. Here we have crafted the interaction (7) between elements so that low order terms in γ recover the exact finite difference formula for linear terms. Note that although centre manifold theory "guarantees" useful properties near the origin in $(u(\xi), \gamma, h)$ space, because of the need to evaluate asymptotic expressions at $\gamma = 1$, we have used a weaker term elsewhere, namely "assures".

3 Numerical comparisons show the effectiveness

We now turn to a detailed description of the centre manifold model for the Kuramoto-Sivashinsky equation (1).

The algebraic details of the derivation of the centre manifold model (11–12) are handled by computer algebra.[1] In an algorithm introduced in [9], the

[1] The REDUCE computer algebra source code is available from the authors upon request.

program iterates to drive to zero the residuals of the governing differential equation (5) and its boundary conditions (6–8). Hence by the Approximation theorems we assuredly construct appropriate approximations to the centre manifold model.

The finite difference model is given by the evolution on the centre manifold. In order to represent the spatial fourth derivative in the Kuramoto-Sivashinsky equation we need to determine the interactions between next-nearest neighbouring elements. Thus the first approximation we can consider involves quadratic terms in γ. After returning to x and t variables it is

$$\begin{aligned}
\frac{du_j}{dt} &= -\frac{\gamma R}{h^2}\left(u_{j+1}-2u_j+u_{j-1}\right)-\frac{\gamma}{2h}u_j(u_{j+1}-u_{j-1})\\
&\quad -\frac{\gamma^2}{h^4}\left(u_{j+2}-4u_{j+1}+6u_j-4u_{j-1}+u_{j-2}\right)\\
&\quad +\frac{\gamma^2 R}{12h^2}\left(u_{j+2}-4u_{j+1}+6u_j-4u_{j-1}+u_{j-2}\right)\\
&\quad +\frac{\gamma^2}{48h}\left(u_{j+2}u_{j+1}+3u_{j+2}u_j-3u_{j+1}-3u_{j+1}u_j\right.\\
&\quad \left.+3u_{j-1}u_j+3u_{j-1}-3u_{j-2}u_j-u_{j-2}u_{j-1}\right)\\
&\quad +\frac{\gamma h^2 u_j^2}{120}\left(u_{j+1}-2u_j+u_{j-1}\right)\\
&\quad +\frac{\gamma^2 h^2}{60480}\left[u_j^2\left(-30u_{j+2}-170u_{j+1}+256u_j-170u_{j-1}-30u_{j-2}\right)\right.\\
&\quad +u_j\left(-126u_{j+2}u_{j+1}-54u_{j+1}u_{j-1}-126u_{j-2}u_{j-1}\right)\\
&\quad \left.+u_{j+1}^2\left(10u_{j+2}-20u_{j+1}+235u_j\right)\right.
\end{aligned}$$

$$+u_{j-1}^2\left(10u_{j-1}-20u_{j-1}+235u_j\right)\Big]$$
$$+\mathcal{O}\left(\|u\|^4,\gamma^3,h^4\right). \tag{13}$$

Recall that $\gamma = 1$ is the case of interest because the internal boundary condition (6–7) evaluated at $\gamma = 1$ ensures sufficient continuity to recover the original problem. The first two lines recorded here, when evaluated for $\gamma = 1$, form the conventional second-order finite difference equation for the Kuramoto-Sivashinsky equation (1). The third line when evaluated for $\gamma = 1$ gives the fourth order accurate corrections to the Ru_{xx} term. The fourth and further lines above start accounting systematically for the variations in the field u within each element and how they affect the evolution through the nonlinear term.

The application of centre manifold theory ensures that the approximation (13) models well the nonlinear dynamics. The finite difference approximation is also independent of any valid rewriting of the PDE because the analysis exploits solutions of the equation not the algebraic form of the equations. Finite difference equations derived via this approach holistically model all the interacting dynamics of the entire PDE.

To show the effectiveness of the approach we compare the finite difference model obtained from various truncations of (13) to accurate numerical solutions obtained on a much finer grid. Choosing m intervals on $[0, 2\pi)$ gives an element length $h = 2\pi/m$ and grid points $x_j = jh$ for $j = 0, \ldots, m-1$. Because of the antisymmetry in $u(x,t)$ about $x = k\pi$, when starting from the initial condition $u(x,0) = 10\sin x$, we only display the interval $[0,\pi]$. There

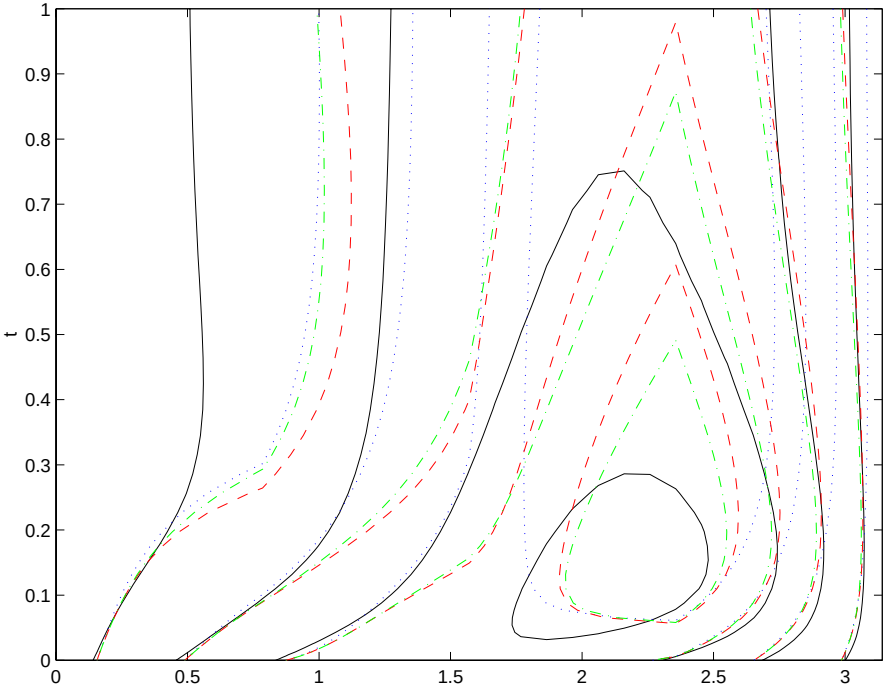

FIGURE 1: Contours of an accurate solution $u(x,t)$, ——, to compare with numerical approximations (13): $\cdots$, the conventional approximation, errors $\mathcal{O}\left(h^2\right)$;– – –, the first correction, errors $\mathcal{O}\left(\|u\|^3\right)$;– · – · – , the second correction,errors $\mathcal{O}\left(\|u\|^4\right)$. Kuramoto-Sivashinsky equation (1) with parameter $R = 2$ is discretised on just $m = 8$ elements in $[0, 2\pi)$ and drawn with contour interval $\Delta u = 3$.

are three different approximations from (13), with $\gamma = 1$, depending upon where the expansion is truncated. The first two lines form a model with $\mathcal{O}(h^2)$ errors (a conventional finite difference approximation), the first five lines provide the first correction with $\mathcal{O}(\|u\|^3)$ errors, and all shown terms form the model with $\mathcal{O}(\|u\|^4)$ errors.

The solutions of these models over $0 < t < 1$ with $m = 8$ and $R = 2$ are shown in Figure 1. Observe that the conventional approximation (dotted) is significantly in error whereas the next two refinements (dot-dashed and dashed) are overall more accurate, especially near the peak. Such accuracy is remarkable considering the nonlinearity, and the few points in the discretisation, $m = 8$.

Figure 2 is a plot of the solution of the models at $t = 1$ with $m = 8$ and $R = 2$. Observe that the conventional approximation undershoots the accurate solution and even has the incorrect sign at $x = \pi/4$. The conventional approximation also overshoots the accurate solution and is particularly poor at $x = 3\pi/4$. Overall the holistic approximations are more accurate than the conventional finite difference approximation.

The solution of the conventional approximation (dotted) and the first holistic correction (dashed) over $0 < t < 1$ with $m = 16$ and $R = 2$ are shown in Figure 3. The second holistic correction was not plotted because it is not discernable from the first correction with $m = 16$. Observe the holistic approximation is again more accurate near the peak.

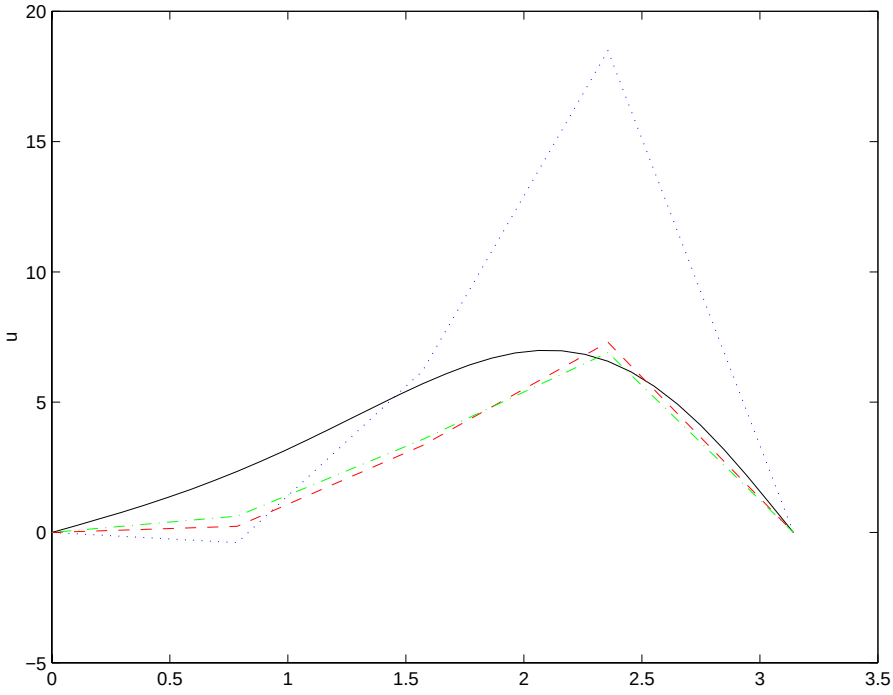

FIGURE 2: Plot of an accurate solution $u(x,t)$, ——, at $t = 1$ to compare with numerical approximations (13):$\cdots$, the conventional approximation, errors $\mathcal{O}\left(h^2\right)$;– – –, the first correction, errors $\mathcal{O}\left(\|u\|^3\right)$;– $\cdot$ – $\cdot$ – , the second correction,errors $\mathcal{O}\left(\|u\|^4\right)$. Kuramoto-Sivashinsky equation (1) with parameter $R = 2$ is discretised on just $m = 8$ elements in $[0, 2\pi)$.

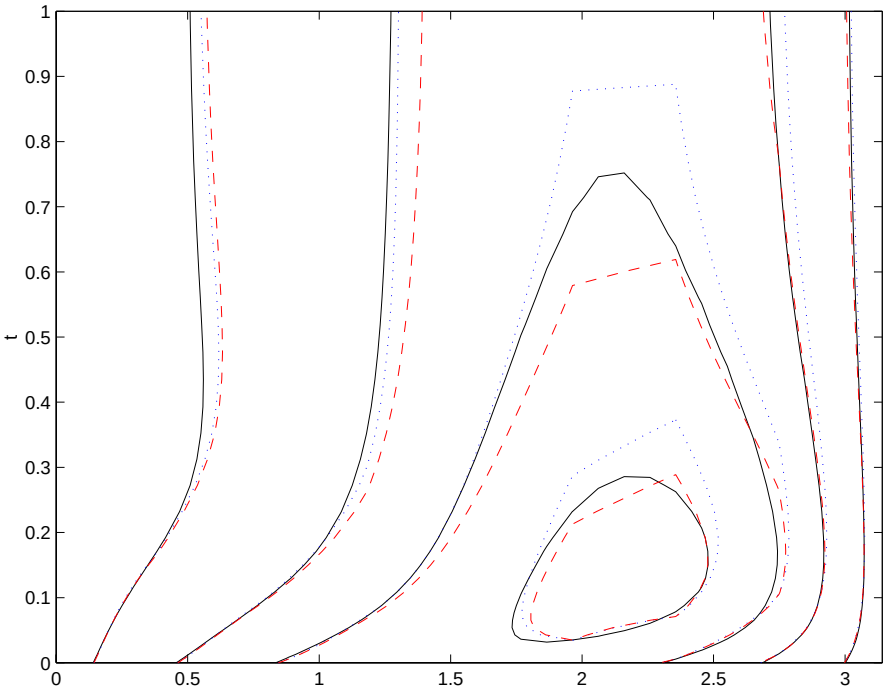

FIGURE 3: Contours of an accurate solution $u(x,t)$, ——, to compare with numerical approximations (13):$\cdots$, the conventional approximation, errors $\mathcal{O}\left(h^2\right)$;– – –, the first correction, errors $\mathcal{O}\left(\|u\|^3\right)$. Kuramoto-Sivashinsky equation (1) with parameter $R = 2$ is discretised on $m = 16$ elements in $[0, 2\pi)$ and drawn with contour interval $\Delta u = 3$.

4 Conclusion

Centre manifold theory is a powerful new approach to deriving finite difference models of dynamical systems. Many details need to researched for a general application of the theory. However, there are many promising features of this application to the Kuramoto-Sivashinsky equation (1) and the earlier example of Burgers' equation [10].

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