Accurately model the Kuramoto–Sivashinsky dynamics with holistic discretisation

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Abstract

We analyse the nonlinear Kuramoto–Sivashinsky equation to develop accurate discretisations modeling its dynamics on coarse grids. The analysis is based upon centre manifold theory so we are assured that the discretisation accurately models the dynamics and may be constructed systematically. The theory is applied after dividing the physical domain into small elements by introducing isolating internal boundaries which are later removed. Comprehensive numerical solutions and simulations show that the holistic discretisations excellently reproduce the steady states and the dynamics of the Kuramoto–Sivashinsky equation. The Kuramoto–Sivashinsky equation is used as an example to show how holistic discretisation may be successfully 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.

Keywords: Kuramoto–Sivashinsky equation, low-dimensional modelling, computational discretisations, multiscale modelling

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1 Introduction

The Kuramoto–Sivashinsky equation, here

\[ \frac{\partial u}{\partial t} + 4 \frac{\partial^4 u}{\partial x^4} + \alpha \left( u \frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2} \right) = 0. \] (1)

was introduced by Sivashinsky [32] as a model of instabilities on interfaces and flame fronts, and by Kuramoto [16] as a model of phase turbulence in chemical oscillations. It receives considerable attention as a model of complex spatio-temporal dynamics [13, 21, 5, 12, e.g.]. In the form (1), with \(2\pi\) periodic boundary conditions, \(\alpha\) is a bifurcation parameter that depends upon the size of the typical pattern [31]. The Kuramoto–Sivashinsky equation includes the mechanisms of linear negative diffusion \(\alpha u_{xx}\), high-order dissipation \(4u_{xxxx}\), and nonlinear advection/steepling \(\alpha uu_x\). The PDE (1) has strong dissipative dynamics arising from the fourth order dissipation. Many modes of this PDE decay rapidly because of this strong dissipation. Thus the dynamics are dominated by a relatively few large scale modes. We create and explore the macroscopic modelling of the Kuramoto–Sivashinsky dynamics using holistic discretisation as initiated by MacKenzie & Roberts [18].

We study the Kuramoto–Sivashinsky equation here for several reasons. Firstly, the PDE is fourth order and therefore, following the example of Burgers’ equation [25], provides a further test case for the application of the holistic approach to higher order dissipative PDEs. Secondly, the Kuramoto–Sivashinsky equation has analogies with the Navier–Stokes equations of fluid dynamics. Holmes, Lumley & Berkooz [12] argued that these analogies exist on two levels: in the energy source and dissipation terms of both dynamical systems; and in the reflection and translational symmetries of the Kuramoto–Sivashinsky equation and
the spanwise symmetries of the Navier–Stokes equations in the boundary layer. This analogy between symmetries suggests the Fourier series and corresponding modal interactions are comparable for these two problems. Thirdly, Cross & Hohenberg [5] describe how the Kuramoto–Sivashinsky equation exhibits the complexities of weak turbulence or spatio-temporal chaos. The complex dynamics of the Kuramoto–Sivashinsky equation (1) is a searching test of the performance of the holistic approach to coarse grained modelling of dynamical systems.

Approximate inertial manifolds and variants [11, 9, 10, 1, 14, e.g.] capture the long-term low dimensional behaviour of the Kuramoto–Sivashinsky equation. Most constructions of approximate inertial manifolds are based upon non-linear Galerkin methods [22, 20, 14, 10, e.g.]. Approximate inertial manifolds are generally constructed by finding global eigenfunctions of the linear dynamics. Our approach is similar to these methods in that we project onto natural solutions of the PDE, and performs nearly as well, see §4.3. But in contrast, the holistic approach undertaken here bases analysis upon the local dynamics within and between finite elements and thus we contend it will be more useful in applications; for example, the approach is readily adapted to the modelling of a wide variety of physical boundary conditions [27].

Our approach is to divide the spatial domain into disjoint elements of finite size $h$ (§2.1). Initially these finite elements are decoupled and so dissipation would cause solutions to exponentially quickly become constant in each element. We then couple the elements together so that information is exchanged between elements—parameterised by a coupling parameter $\gamma$ so that $\gamma = 1$ recovers the original Kuramoto–Sivashinsky dynamics. The coupling drives the evolution of the field in each element. Solving the Kuramoto–Sivashinsky PDE within each element, and with the inter-element coupling, hence resolves subgrid scale dynamics and their interactions with nearby elements. Crucially, such solutions are determined in constructing the holistic model and so are done only once; the holistic model may then be used many times without any further analysis of subgrid structure as the subgrid structure has already been incorporated into the closure of the holistic model. Centre manifold theory [3, 23, e.g.] provides the rigorous support for holistic models as introduced by Roberts [25] for Burgers’ equation and discussed in §2.2.

For example, a low order analysis, reported in §3.1, of the Kuramoto–Sivashinsky equation (1) favours the discretisation

$$\frac{du_j}{dt} + \frac{4u_{j+2} - 16u_{j+1} + 24u_j - 16u_{j-1} + 4u_{j-2}}{h^4}$$
where the \( u_j \)'s are grid values spaced \( h \) apart (one for each element). The first two lines of the holistic discretisation (2) shows the holistic method generates conventional centered finite difference approximations for the linear terms \( 4u_{xxxx} \) and \( \alpha u_{xx} \). The third line details a specific nonstandard approximation for the nonlinear term \( \alpha uu_x \): it is a mix of three valid approximations to \( uu_x \); the holistic analysis determines the specific mix through the subgrid scale modelling of physical processes, see §3.2. The holistic discretisation is not constructed by discretising the Kuramoto–Sivashinsky equation (1) term by term, rather the subgrid scale dynamics of (1) together with inter-element coupling generate the specific holistic discretisation (2).

The discretisation (2) is a low-order approximation. Centre manifold theory provides systematic refinements. Analysis of the centre manifold to higher orders in nonlinearity or inter-element interaction, discussed in §3, gives further refinement to the discretisation. The higher order terms come from resolving more subgrid scale processes and interactions. One effect of resolving systematically the interactions between elements is that the holistic model and the PDE agree to high order in the element size \( h \): for example, the low order model (2) is equivalent to the PDE

\[
\frac{\partial u}{\partial t} = -\alpha \left( u \frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2} \right) - 4 \frac{\partial^4 u}{\partial x^4} - \frac{2h^2}{3} \frac{\partial^6 u}{\partial x^6} + O(h^4),
\]

as \( h \to 0 \). Thus the nonlinear processes are modelled with an error that decreases quadratically to zero with element size. Further higher order analyses lead to higher order consistency, as element size \( h \to 0 \), between the equivalent PDEs, such as (3), of the holistic discretisations and the Kuramoto–Sivashinsky PDE (see §3.3). Such consistency is further justification for our approach in addition to the support provided by centre manifold theory for finite element size \( h \).

The bulk of this paper is then a comprehensive comparative study of the various models of the Kuramoto–Sivashinsky dynamics; even further details are reported by MacKenzie [19]. A detailed numerical study of the holistic predictions for the steady states of the Kuramoto–Sivashinsky equation is the focal point of Section 4, followed by an exploration of the holistic predictions.
for the time dependent phenomena of the Kuramoto–Sivashinsky equation in Section 5. We compare: the predicted steady states, their stability and bifurcation diagrams; the dynamics near the steady states; Hopf bifurcations leading to period doubling sequences; and the spatio-temporal patterns at relatively large nonlinearity parameter $\alpha$. We find that the holistic models have excellent performance on coarse grids thus enabling simulations to use large time steps. The excellent performance detailed herein is further evidence that the holistic approach is a robust and useful method for discretising PDEs.

2 Use a homotopy in inter-element coupling

The construction of a discretisation is based upon breaking the spatial domain into disjoint finite elements and then joining them together again. We control this process by a coupling parameter $\gamma$ that smoothly parametrises the transition between decoupled elements and fully coupled elements for which we recover a model for the original PDE. Furthermore, we construct the model using solutions of the PDE within each element and hence resolve subgrid scale dynamics. Centre manifold theory [3, 23, e.g.] provides the rigorous support for holistic models as introduced by Roberts [25] for Burgers’ equation.

2.1 Introduce internal boundaries between elements

Establish the spatial discretisation by dividing the domain into $m$ elements of equal and finite width $h$ and introducing an equispaced grid of collocation points, $x_j = jh$, at the centre of each element, see Figure 1.\footnote{In principle, elements may be of unequal size. However, to simplify the analysis, herein all elements are of equal width $h$.} Express the
subgrid field in the jth element by \( u = v_j(x, t) \) — we solve the Kuramoto–Sivashinsky PDE (1) with inter-element coupling introduced via artificial internal boundary conditions (IBCs). We introduce a homotopy in an inter-element coupling parameter \( \gamma \): when \( \gamma = 0 \) the elements are effectively isolated from each other, providing the basis for the application of centre manifold theory; whereas when evaluated at \( \gamma = 1 \) the elements are fully coupled together and hence the discretised model applies to the original PDE. Since the Kuramoto–Sivashinsky PDE is fourth order we require four IBCs for each element to ensure satisfactory coupling between neighbouring elements. Here we use the non-local IBCs

\[
\delta_x v_j(x, t) = \gamma \delta v_{j\pm 1/2}(x, t) \quad \text{at} \quad x = x_{j\pm 1/2}, \tag{4}
\]

\[
\delta_x^3 v_j(x, t) = \gamma^2 \delta^3 v_{j\pm 1/2}(x, t) \quad \text{at} \quad x = x_{j\pm 1/2}, \tag{5}
\]

which are an extension of the non-local IBCs explored by Roberts [26] for Burgers’ equation; alternative local IBCs were explored by MacKenzie [19] but are generally inferior. The non-local IBCs (4–5) involve the centered difference operators \( \delta \) and \( \delta_x \); the operator \( \delta_x \) denotes a centered difference in \( x \) only, with step \( h \); whereas the operator \( \delta \) denotes a centered difference applied to the grid index \( j \) with step 1; so for example, the first of the IBCs, (4), is

\[
v_j(x_{j\pm 1}, t) - v_j(x_j, t) = \gamma [v_{j+1}(x_{j\pm 1}, t) - v_j(x_j, t)]. \tag{6}
\]

Note: the field \( v_j(x, t) \) extends analytically to at least \( x_{j\pm 2} \) to allow the application of the non-local IBCs (5). The physical interpretation of these IBCs is not obvious. Firstly, when \( \gamma = 0 \), (4–5) ensures the first and third differences in \( x \) of the field \( v_j \) centered about the element boundaries \( x_{j\pm 1/2} \) are zero. These isolate each element from its neighbours as there is then no coupling between them. In each element \( v_j(x, t) = \text{constant} \) is an equilibrium. It is dynamically attractive provided the instability controlled by \( \alpha/h^2 \) is not too large compared with the dissipation of order \( 1/h^4 \). This simple class of piecewise constant solutions provide the basis for analysing the dynamics when the elements are coupled together with non-zero \( \gamma \). Secondly, the non-local IBCs evaluated at \( \gamma = 1 \) requires that the field \( v_j(x, t) \), when extrapolated to \( x_{j\pm 1} \) and \( x_{j\pm 2} \), is to equal the grid point value of the subgrid field of that element, \( u_{j\pm 1} \) and \( u_{j\pm 2} \) respectively. See the schematic representation in Figure 2 of these non-local boundary conditions evaluated at \( \gamma = 1 \). This requirement restores sufficient continuity to ensure the holistic model applies to the original PDE.

The inter-element coupling parameter \( \gamma \) controls the flow of information between neighbouring elements. We construct solutions as power series expansions

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in the coupling parameter $\gamma$\footnote{Such homotopies are used successfully in other numerical methods. For example, Liao\cite{17} proposed a homotopy in his general boundary element method from auxiliary linear operators whose fundamental solutions are well known. Here the homotopy is only in the \textsc{iBC}s.}. When $O(\gamma^2)$ terms are neglected in the holistic model, the field in the $j$th element involves information about the fields in the $j \pm 1$ elements. Similarly, when $O(\gamma^3)$ terms are neglected in the approximation, the field in the $j$th element involves information about the fields in the $j \pm 1$ and $j \pm 2$ elements. Consequently, the order of $\gamma$ retained in the holistic model controls the stencil width of the discretisation.

Roberts\cite{26} argued that this particular form of the non-local \textsc{iBC}s ensures that these holistic models are consistent with any given \textsc{PDE} to high orders in the grid size $h$ as $h \to 0$. Interestingly, Roberts & Kevrekidis\cite{29} show that closely related coupling boundary conditions provide high order consistency for multiscale simulations using the gap-tooth scheme.

### 2.2 Centre manifold theory supports the discretisation

The existence, relevance and approximation theorems [3, 4, e.g.] of centre manifold theory apply to the Kuramoto–Sivashinsky \textsc{pDE} (1) with \textsc{iBC}s (4–5). Similar to the application to Burgers’ equation by Roberts\cite{25}, the result here is support for a low dimensional discrete model for the Kuramoto–Sivashinsky dynamics at finite grid size.

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![Figure 2: Schematic diagram of the fields $v_j(x,t)$, $v_{j+1}(x,t)$ and $v_{j-1}(x,t)$ for the non-local \textsc{iBC}s (4–5) with $\gamma = 1$. See the fields pass through neighbouring grid values $u_j$ and $u_{j\pm1}$, and also $u_{j\pm2}$ when appropriate.](image)

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Theoretical support is based upon the piecewise constant solutions obtained when all the elements are insulated from each other. Adjoin to the Kuramoto–Sivashinsky PDE (1) the dynamically trivial equations for the coupling parameter $\gamma$ and the nonlinearity parameter $\alpha$, 
\[ \frac{\partial \gamma}{\partial t} = \frac{\partial \alpha}{\partial t} = 0, \]
and consider the dynamics in the extended state space $(u(x), \gamma, \alpha)$. Adjoining such trivial equations for parameters is commonly used to unfold bifurcations \cite[§1.5]{3}. In this extended space there is a subspace of fixed points with $u = \text{constant}$ in each element and $\gamma = \alpha = 0$.\footnote{In principle we need not base the analysis about a zero nonlinearity parameter. In practise, allowing non-zero $\alpha$ as a base makes the algebra too complicated as the subgrid structure would then be determined by recursively solving equations of the form $-4u''_{xxxx} - \alpha(u''_{xx} + u_j u'_x) = \text{rhs}$ for corrections $u'$. Thus the practical route for this modelling of nonlinear PDEs is to adjoin $\partial \alpha/\partial t = 0$ so we treat the nonlinear parameter $\alpha$ as small.} Linearising the PDE and IBCS about each fixed point, $u = \text{constant} + u'(x, t)$ for small $u'$, gives 
\[ \frac{\partial u'}{\partial t} = -\frac{\partial^4 u'}{\partial x^4} \quad \text{such that} \quad \delta_x u'(x, t)|_{x=x_{j\pm 1/2}} = \delta^3_x u'(x, t)|_{x=x_{j\pm 1/2}} = 0. \]
Solving these linear equations, the $n$th linear eigenmode associated with each element is 
\[ \alpha = \gamma = 0, \quad u' \propto e^{\lambda_n t} \cos \left[ \frac{n\pi}{h} (x - x_{j-1/2}) \right], \]
for the non-local IBCS (4–5), where $n = 0, 1, 2, \ldots$ and the eigenvalue $\lambda_n = -n^4 \pi^4 / h^4$. There are also the trivial modes $\gamma = \text{const}$ and $\alpha = \text{const}$. Therefore, in a spatial domain of $m$ elements there are $m + 2$ zero eigenvalues: one associated with each of the $m$ elements; and two from the trivial (7). All other eigenvalues are negative, $\leq -\pi^4 / h^4$. Thus, the existence theorem, see \cite[p.281]{4} or \cite[p.96]{33}, guarantees that a $m + 2$ dimensional centre manifold $\mathcal{M}$ exists for the Kuramoto–Sivashinsky PDE (1) with the trivial (7) and IBCS (4–5).

We parametrise the $(m + 2)$ dimensional centre manifold $\mathcal{M}$ by the $m + 2$ parameters $\gamma, \alpha$ and the grid values $u_j$.\footnote{These grid values are one choice to represent the magnitude of the field $u$ in each element. Other choices to represent the local field are possible, but the grid values appear most convenient.} Denote $u$ as the vector of the $m$ grid values. Thus for some function $v$ to be determined the centre manifold $\mathcal{M}$ is 
\[ u(x, t) = v(x; u, \gamma, \alpha). \]
However, we find it convenient to view the centre manifold (9) as the union of the set of subgrid fields $v_j(x; u, \gamma, \alpha)$ over the physical domain. The corresponding
amplitude condition, that the field in each element has to pass through its grid value, is
\[ u_j = v_j(x_j; u, \gamma, \alpha). \] (10)

The existence theorem [4] also asserts that on the centre manifold the grid values \( u_j \) evolve deterministically in time according to the system of ODEs
\[ \dot{u}_j = du_j/dt = g_j(u, \gamma, \alpha), \] (11)
where \( g_j \) is the restriction of the Kuramoto–Sivashinsky PDE (1) with the trivial (7) and BCs (4–5) to the centre manifold \( \mathcal{M} \). It is this evolution (11) of the grid values that gives the holistic discretisation.

Note that the centre manifold \( \mathcal{M} \) is global in \( u \) but local in \( \gamma \) and \( \alpha \). When the parameters \( \gamma = \alpha = 0 \) the Kuramoto–Sivashinsky PDE has an \( m \) dimensional centre subspace \( \mathcal{E} \) of fixed points with the field \( u \) being independently constant in each element; these are fixed points for all \( u \). When the parameters \( \gamma \) and \( \alpha \) are non-zero this subspace is “bent” to the curved centre manifold \( \mathcal{M} \). Thus the models we construct are valid for small enough \( \gamma \) and \( \alpha \), although we use them at finite \( \gamma \) and \( \alpha \), but are formally valid for all \( |u| \). Numerical solutions of the centre manifold models, such as those in §3.2, indicate that parameter values as large as \( \gamma = 1 \) and \( \alpha = 20–50 \) are indeed within the range of validity of our approach, even on relatively coarse grids.

We now support the claim that the evolution of the discrete grid values (11) actually models the Kuramoto–Sivashinsky PDE (1). The relevance theorem of centre manifolds, [4, p.282] or [33, p.128], guarantees that all solutions of the Kuramoto–Sivashinsky PDE (1) with (7) and the BCs (4–5), which remain in some neighbourhood of the centre subspace \( \mathcal{E} \) in \((u(x), \gamma, \alpha)\) space are exponentially quickly attracted to the centre manifold \( \mathcal{M} \) and thence to a solution of the \( m \) discrete ODEs (11). For our application of centre manifold theory to the holistic model we seek regimes where this neighbourhood includes \( \gamma = 1 \) and \( \alpha \) of interest. We estimate the rate of attraction by the leading negative eigenvalue, here \( \lambda_1 = -\pi^4/h^4 \). The actual rate of attraction may be less due to the difference between centre manifold \( \mathcal{M} \) and the centre subspace \( \mathcal{E} \), but \( \lambda_1 \) is the correct order of magnitude. This exponentially quick attraction ensures the so-called asymptotic completeness [30]: after the exponentially quick transients of the approach to \( \mathcal{M} \) by any trajectory, the evolution of the discretisation (11) on \( \mathcal{M} \) accurately models the dynamics of the Kuramoto–Sivashinsky PDE (1).
2.3 Approximate the shape of the centre manifold

Having established that we may find a low dimensional description (9–11) of the interacting elements that is relevant to the Kuramoto–Sivashinsky PDE (1), we need to construct the shape of centre manifold and the corresponding evolution on the manifold. The approximation theorem of Carr & Muncaster [4, p.283] assures us that upon substituting the ansatz (9–11) into the complete system and solving to some order of error in $\alpha$ and $\gamma$, then the centre manifold $\mathcal{M}$ and the evolution thereon will be approximated to the same order. However, we need to evaluate the approximations at the coupling parameter $\gamma = 1$ because it is only then that the artificial internal boundaries are removed. Thus the actual error of the model due to the evaluation at $\gamma = 1$ is not estimated. However, the holistic method for discretising the Kuramoto–Sivashinsky equation is supported three ways: firstly, the smooth homotopy from $\gamma = 0$ with large spectral gap to the gravest decaying mode with decay rate $\approx -\pi^4/h^4$; secondly the holistic models are consistent with the Kuramoto–Sivashinsky PDE to high order in grid size $h$, see §3.3; thirdly, we see in Sections 4–5 that the holistic discretisation resolves accurately both steady state solutions and time dependent phenomena of the Kuramoto–Sivashinsky PDE.

To construct the centre manifold, we solve for the field $v_j$ in each element. For definiteness, here we consider domains periodic in space, or equivalently elements far from the influence of any physical boundary. By translational symmetry of the Kuramoto–Sivashinsky PDE (1) the subgrid field in each element is identical, except for the appropriate shift in the grid index $j$. Thus, we construct the subgrid field and evolution for a general $j$th element; Section 3 gives some examples.

The algebraic details of the derivation of the centre manifold model (9–11) are handled by computer algebra. In an algorithm introduced by Roberts [24], iteration drives to zero the residuals of the governing PDE (1) and its ibcs (4–5) and amplitude condition (10). Since the algebraic details of the construction are tedious, they are not given; instead see the computer algebra procedure of [28].

This computer algebra is based upon driving the residuals of the governing equations to zero in the following manner. Recall from §2.2 that the grid values $u$ parametrise the centre manifold (9) and that (11) gives the evolution of the grid values. Thus substitute these into the Kuramoto–Sivashinsky PDE (1) and seek to solve

$$\frac{\partial v_j}{\partial t} = \sum_k \frac{\partial v_j}{\partial u_k} g_k = -4 \frac{\partial^4 v_j}{\partial x^4} - \alpha \left( \frac{\partial^2 v_j}{\partial x^2} + v_j \frac{\partial v_j}{\partial x} \right), \quad (12)$$
Use a homotopy in inter-element coupling

together with the non-local IBCs (4–5) and the amplitude equation (10), to some order in parameters $\gamma$ and $\alpha$. The iteration is that given any approximation, denoted by $\tilde{v}$, we seek corrections, denoted by primes, such that $v_j = \tilde{v}_j + v'_j$ and $g_j = \tilde{g}_j + g'_j$, better satisfy the Kuramoto–Sivashinsky PDE. Thus in each iteration we solve a problem of the form,

$$-4 \frac{\partial^4 v'_j}{\partial x^4} = g'_j + \text{Residual}, \tag{13}$$

where from (12) the

$$\text{Residual} = \sum_k \frac{\partial \tilde{v}_j}{\partial u_k} g_k + 4 \frac{\partial^4 \tilde{v}_j}{\partial x^4} + \alpha \left( \frac{\partial^2 \tilde{v}_j}{\partial x^2} + \tilde{v}_j \frac{\partial \tilde{v}_j}{\partial x} \right), \tag{14}$$

together with the IBCs, for the corrections, primed quantities, to the subgrid field and the evolution of the grid values. Note: the residual in (14) is the residual of the Kuramoto–Sivashinsky PDE for the current approximation. The iteration scheme starts with the linear solution in each element, namely $v_j(x, u, \gamma, \alpha) = u_j$ and $g_j(u, \gamma, \alpha) = 0$. The iteration terminates when the residuals of the Kuramoto–Sivashinsky PDE (12), and the IBCs, are zero to some order in ($\gamma, \alpha$). Then theory assures us that the subgrid field in each element and the evolution of the grid values are correct to the same order in ($\gamma, \alpha$); that is, when the residuals are of order $O(\gamma^m, \alpha^n)$, theory assures us the errors are also of order $O(\gamma^m, \alpha^n)$. This assurance holds for both steady states and for time dependent dynamics.

3 Various holistic models

Here we record holistic models of the Kuramoto–Sivashinsky PDE (1), to various orders in coupling parameter $\gamma$, governing the width of the numerical stencil, and in the nonlinearity parameter $\alpha$. In order to be used the models need to be evaluated at $\gamma = 1$ as then the non-local IBCs (4–5) ensure sufficient continuity in the solution field. We write the models in terms of the centered difference and mean operators,

$$\delta u_j = u_{j+1/2} - u_{j-1/2} \quad \text{and} \quad \mu u_j = (u_{j+1/2} + u_{j-1/2})/2,$$

respectively. A REDUCE program [28] constructs all models. We only present in detail here holistic models to errors $O(\alpha^2)$ as the level of complexity increases enormously with the order of nonlinearity $\alpha$.
3.1 Some holistic discretisations

In order to represent the spatial fourth derivative in the Kuramoto–Sivashinsky equation, we need at least a 5 point stencil approximation. Thus we determine the interactions between at least next-nearest neighbouring elements by obtaining up to at least quadratic terms in the coupling parameter $\gamma$. Computer algebra readily determines higher order expressions in the coupling parameter $\gamma$:

$$\dot{u}_j = -\frac{\gamma \alpha}{h^2} \delta^2 u_j - \frac{\gamma \alpha}{h} u_j \delta \mu u_j - \frac{4 \gamma^2}{h^4} \delta^4 u_j + \frac{\gamma^2 \alpha}{12h^2} \delta^4 u_j$$

$$+ \frac{\gamma^2 \alpha}{12h} (2u_j \delta^3 \mu u_j + \delta^2 u_j \delta^3 \mu u_j + \delta^4 u_j \delta \mu u_j)$$

$$+ \frac{2 \gamma^3}{3h^4} \delta^6 u_j - \frac{\gamma^3 \alpha}{90h^2} \delta^6 u_j$$

$$- \frac{\gamma^3 \alpha}{480h} \left(16u_j \delta^5 \mu u_j + 30 \delta^4 u_j \delta^3 \mu u_j + 40 \delta^2 u_j \delta^3 \mu u_j + 40 \delta^4 u_j \delta \mu u_j + 78^4 u_j \delta^5 \mu u_j + 78^6 \delta^3 \mu u_j\right)$$

$$- \frac{7 \gamma^4}{60h^4} \delta^8 u_j + \frac{\gamma^4 \alpha}{560h^2} \delta^8 u_j$$

$$+ \frac{\gamma^4 \alpha}{60480h} \left(432u_j \delta^7 \mu u_j + 3528 \delta^2 u_j \delta^5 \mu u_j + 1507 \delta^2 u_j \delta^7 \mu u_j + 3780 \delta^4 u_j \delta^5 \mu u_j + 3951 \delta^4 u_j \delta^5 \mu u_j + 984 \delta^4 u_j \delta^7 \mu u_j + 1764 \delta^6 u_j \delta^5 \mu u_j + 3419 \delta^6 u_j \delta^3 \mu u_j + 1414 \delta^6 u_j \delta^5 \mu u_j + 164 \delta^6 u_j \delta^7 \mu u_j + 523 \delta^8 u_j \delta^5 \mu u_j + 656 \delta^8 u_j \delta^3 \mu u_j + 164 \delta^8 u_j \delta^5 \mu u_j\right) + O(\gamma^5, \alpha^2).$$

We have ordered (and coloured) the terms in this discretisation in increasing powers of coupling parameter $\gamma$ in order to discuss the three different truncations labelled by the three different equation numbers.

**The $O(\gamma^3, \alpha^2)$ holistic discretisation** is formed by truncating the above model to the (green) terms before and at (15). Evaluated at coupling parameter $\gamma = 1$ this discretisation forms the basic 5 point stencil approximation (2) discussed in the Introduction. The first line of (15), when evaluated at $\gamma = 1$, gives a second order centered difference approximation for the hyperdiffusion term $4u_{xxxx}$, a fourth order centered difference approximation to the linear growth term $\alpha u_{xx}$, and a second order centered difference approximation to
the nonlinear advection term $\alpha u u_x$. The second line modifies the nonlinear discretisation to account for interaction with nonlinear effects caused by the next-nearest neighbour elements.

The holistic discretisation (15) contains the approximation

$$u u_x|_{x_j} \approx \left( u_j \frac{u_{j+1} - u_{j-1}}{4h} + \frac{u_{j+1}^2 - u_{j-1}^2}{4h} - \frac{u_{j+2} u_{j+1} - u_{j-2} u_{j-1}}{12h} \right).$$

(18)

when evaluated at $\gamma = 1$. This is a $1/2 : 1 : -1/2$ mix of the approximations

$$u u_x|_{x_j} \approx u_j \frac{u_{j+1} - u_{j-1}}{2h} \approx \frac{u_{j+1}^2 - u_{j-1}^2}{4h} \approx \frac{u_{j+2} u_{j+1} - u_{j-2} u_{j-1}}{6h},$$

(19)

respectively. This particular nonstandard approximation (18) to the nonlinear term $\alpha u u_x$, arises due to the modelling of subgrid scale interactions between the Kuramoto–Sivashinsky equation and the inter-element coupling. Such nonstandard approximations generated through this approach can have robust numerical characteristics [26, §2].

**The $\mathcal{O}(\gamma^4, \alpha^2)$ holistic discretisation** is formed by truncating the above model to the (green and olive green) terms before and at (16). This discretisation forms a 7 point stencil approximation, involving $u_j, u_{j\pm 1}, u_{j\pm 2}$ and $u_{j\pm 3}$. The first and third lines of (16), when evaluated at $\gamma = 1$, give a fourth order centered difference approximation to the hyperdiffusion term, a sixth order centered difference approximation to the linear growth term, and a second order centered difference approximation to the nonlinear advection term. The second, fourth, fifth and sixth lines account for higher order subgrid scale dynamics of the nonlinearity and its inter-element coupling to generate a fourth order centered difference approximation to the nonlinearity $u u_x$.

**The $\mathcal{O}(\gamma^5, \alpha^2)$ holistic discretisation** (17) (all coloured terms) forms a 9 point stencil approximation, involving only $u_j, u_{j\pm 1}, u_{j\pm 2}, u_{j\pm 3}$ and $u_{j\pm 4}$. The first, third and seventh lines of (17) when evaluated at $\gamma = 1$ give a sixth order centered difference approximation for the hyperdiffusion term, an 8th order centered difference approximation for the linear growth term and a second order centered difference approximation for the nonlinear advection term. The remaining lines provide modifications to model the nonlinear $u u_x$ to sixth order through resolving subgrid scale dynamics.

We do not code these discretisations manually. Instead, the computer algebra program at [28] is used with the UNIX editor *sed* to automatically write the discretisation in a form suitable for MATLAB simulation.
Various holistic models

Compare with conventional centered difference models. Traditional direct finite differences generate the following discretisation of the Kuramoto–Sivashinsky PDE (1):

\[ \dot{u}_j = -\frac{\alpha}{h} u_j \delta \mu u_j - \frac{\alpha}{h^2} \delta^2 u_j - \frac{4}{h^4} \delta^4 u_j \]

(20)

\[ + \frac{\alpha}{h^6} u_j \delta^3 \mu u_j + \frac{\alpha}{h^2 12} \delta^4 u_j + \frac{4}{h^4 6} \delta^6 u_j \]

(21)

\[ - \frac{\alpha}{h 30} u_j \delta^5 \mu u_j - \frac{\alpha}{h^2 90} \delta^6 u_j - \frac{4}{h^4 7} \frac{1}{240} \delta^6 u_j + \mathcal{O}(h^6) \]  

(22)

Truncate the above discretisation to the terms before and at

- (20) to obtain a 5 point conventional discretisation;
- (21) to obtain a 7 point conventional discretisation;
- (22) to obtain a 9 point conventional discretisation.

Consider the different view of the errors for the discretisations: the centered difference approximations (20–22) are justified by consistency as grid size \( h \to 0 \); whereas the holistic discretisations (15–17) are supported by centre manifold theory at finite grid size \( h \). The errors in the centre manifold approach are due to the truncation of dependence in the inter-element coupling parameter \( \gamma \) and the nonlinearity parameter \( \alpha \). However, as argued by Roberts [26] for linear systems and as demonstrated in §3.3, the particular choice of the IBCs (4–5) ensures that the holistic discretisations are also consistent as \( h \to 0 \) with the Kuramoto–Sivashinsky PDE (1).

3.2 Modelling the subgrid field powers our methodology

Recall that the set of subgrid fields over the physical domain form a state on the centre manifold. Here we plot some example subgrid fields for various holistic models. For example, Figure 3 shows the evolving subgrid fields of wave like solutions of the holistic discretisation (15) compared with an accurate solution and the Lagrangian interpolation of the second order centred difference model (20). Such plots reinforce the link between the abstract centre manifold description of the dynamics and the physical subgrid fields for the low order holistic models. Recall that the key methodology difference with conventional finite differences, and finite elements, is that the subgrid fields of the holistic
models are constructed by actual local solutions of the Kuramoto–Sivashinsky PDE, see §2.3.

Until Section 5 we restrict attention to odd symmetric solutions that are $2\pi$ periodic. This restriction is to compare results with the numerical investigations of Jolly et al. [14] which we consider in more detail in Sections 4 and 5. Typically we use a grid of 8 equi-spaced elements on the interval $[0, \pi]$. The sub-grid fields are plotted for approximations to the steady states of the Kuramoto–Sivashinsky equation (1) with these periodic boundary conditions, computed using holistic discretisations at the high values of the nonlinearity parameter $\alpha = 20$ and $\alpha = 50$.  

Figure 3: $\alpha = 5$: wave like solutions at $t = 0, 0.2, 0.4, 0.6, 0.8, 1$ for the $O(\gamma^3, \alpha^2)$ holistic model (15) shown in green and the second order centered difference approximation (20) in magenta on a coarse grids of 8 elements on $[0, 2\pi]$. The accurate solution is shown in blue.
Higher order holistic models improve the accuracy and continuity of the subgrid field. Figure 4 displays the subgrid fields of three holistic models for a steady state of the Kuramoto–Sivashinsky PDE for $\alpha = 20$. Observe the collection of subgrid fields forms the field $u$ which is a state on the centre manifold. The $O(\gamma^3, \alpha^2)$ holistic model (15) (green) is the least accurate and has the largest jump at element boundaries. But note that Lagrangian interpolation of the steady state of the second order conventional approximation (20) is significantly less accurate [19]. The $O(\gamma^4, \alpha^2)$ (16) model (olive green) displays improvement over the holistic $O(\gamma^3, \alpha^2)$ approximation. The $O(\gamma^5, \alpha^2)$ (17) model (cyan) is the most accurate, being almost indistinguishable from the correct solution.

Figure 5 shows a steady state of the Kuramoto–Sivashinsky PDE at $\alpha = 50$. The accurate field is symmetric (blue curve). For this value of the nonlin-
Figure 5: Subgrid fields of the holistic models with errors $O(\gamma^3, \alpha^2)$ (15) (green), $O(\gamma^4, \alpha^2)$ (16) (olive green) and $O(\gamma^5, \alpha^2)$ (17) (cyan), for a steady state of the Kuramoto–Sivashinsky equation at $\alpha = 50$, with 8 elements on $[0, \pi]$. An accurate solution is also plotted in blue.

earity there is no steady state solution for centered difference approximations of either second (20), fourth (21) or sixth order (22) on this coarse grid of 8 elements on $[0, \pi]$. However, the 5 point stencil holistic approximation with errors $O(\gamma^3, \alpha^2)$ (15) (green) models this steady state of the Kuramoto–Sivashinsky equation even for such a large value of the nonlinearity on this coarse grid. This $O(\gamma^3, \alpha^2)$ holistic solution has significant jumps across the subgrid field at element boundaries; moreover, the subgrid field is not symmetric and is most inaccurate near the centre of the spatial domain considered here. The 7 point stencil holistic approximation with errors $O(\gamma^4, \alpha^2)$ (16) (olive green) is more accurate with smaller jumps between neighbouring the subgrid fields, but is also not symmetric. The 9 point stencil holistic approximation with errors $O(\gamma^5, \alpha^2)$ (17) (cyan) is the most accurate of the holistic models illustrated here; it is symmetric and the jumps between neighbouring subgrid fields are
These illustrations of the subgrid fields of steady states of the Kuramoto–Sivashinsky equation at $\alpha = 20$ and $\alpha = 50$ indicate the holistic models perform well even at such large values of a supposedly small parameter. The performance of the holistic models are explored further in Section 4 for steady states and Section 5 for time dependent phenomena.

3.3 The holistic discretisations are consistent

Holistic models constructed by implementing the IBCS (4–5) have dual justification [26]: they are supported by centre manifold theory for small enough $\alpha$ and $\gamma$; as well as being justified by their consistency as the grid size $h \to 0$. We explore consistency as a well established feature of numerical analysis.\(^5\)

Here we examine the equivalent PDEs for the holistic discretisations (15–17) evaluated at $\gamma = 1$, and the centered difference approximations (20–22). These equivalent PDEs establish the $O(h^{2p-2})$ consistency with the Kuramoto–Sivashinsky PDE for holistic models constructed with residuals $O(\gamma^{p+1})$.

Roberts [26] proved that using IBCS of the form introduced in §2 and retaining terms up to $\gamma^p$ in the holistic approximations results in approximations which are consistent with the linear terms of the Kuramoto–Sivashinsky equation (1) to $O(h^{2p-2})$, provided $p \geq 2$. However, accumulating evidence indicates the IBCS (4–5) also ensure $O(h^{2p-2})$ consistency for the nonlinear dynamics. As yet no formal proof exists of this nonlinear consistency, but all holistic models of the Kuramoto–Sivashinsky equation, containing terms up to $\gamma^7$ and $\alpha^4$ and constructed using (4–5) are nonlinearly consistent (although not all are recorded here).

Find the equivalent PDEs for the various discretisations by expanding the discretisations in grid size $h$ about a grid point $x_j$. That is, write

$$u_{j \pm m} = u_j \pm mh \frac{\partial u_j}{\partial x} + m^2 \frac{h^2}{2} \frac{\partial^2 u_j}{\partial x^2} + \sum_{k=3}^{\infty} (\pm m)^k \frac{h^k}{k!} \frac{\partial^k u_j}{\partial x^k}, \quad (23)$$

to whatever order in $h$ is required. Computer algebra performs the tedious details. As for the example equivalent PDE (3), all equivalent PDEs have the form

$$\frac{\partial u}{\partial t} = -\alpha \left( u \frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2} \right) - 4 \frac{\partial^4 u}{\partial x^4} + E, \quad (24)$$

\(5\)But note that high order consistency is not a primary goal of this holistic approach, since we aim to develop and support models for finite element size $h$. 

Tony Roberts, November 22, 2006
### Table 1: errors $E$ of the equivalent PDE of holistic and conventional discretisations, see (24). MacKenzie [19] gave more details.

<table>
<thead>
<tr>
<th>stencil</th>
<th>holistic (15–17)</th>
<th>conventional (20–22)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 point</td>
<td>$-\frac{2h^2}{3} \frac{\partial^6 u}{\partial x^6} + \mathcal{O}(h^4)$</td>
<td>$-h^2 \left( \frac{\alpha}{3} \frac{\partial^3 u}{\partial x^3} \frac{\partial u}{\partial x} + \frac{\alpha}{12} \frac{\partial^3 u}{\partial x^3} + \frac{2}{3} \frac{\partial^6 u}{\partial x^6} \right) + \mathcal{O}(h^4)$</td>
</tr>
<tr>
<td>7 point</td>
<td>$-\frac{7h^4}{60} \frac{\partial^8 u}{\partial x^8} + \mathcal{O}(h^6)$</td>
<td>$-h^4 \left( \frac{\alpha}{50} \frac{\partial^5 u}{\partial x^5} \frac{\partial u}{\partial x} + \frac{\alpha}{90} \frac{\partial^6 u}{\partial x^6} + \frac{7}{60} \frac{\partial^8 u}{\partial x^8} \right) + \mathcal{O}(h^6)$</td>
</tr>
<tr>
<td>9 point</td>
<td>$-\frac{41h^6}{1890} \frac{\partial^{10} u}{\partial x^{10}} + \mathcal{O}(h^8)$</td>
<td>$-h^6 \left( \frac{\alpha}{140} \frac{\partial^7 u}{\partial x^7} \frac{\partial u}{\partial x} + \frac{\alpha}{560} \frac{\partial^8 u}{\partial x^8} + \frac{41}{1890} \frac{\partial^{10} u}{\partial x^{10}} \right) + \mathcal{O}(h^8)$</td>
</tr>
</tbody>
</table>

where $E$ denotes the error between the equivalent PDE of the discretisation and the Kuramoto–Sivashinsky PDE (1). Table 1 lists the errors for the holistic discretisations (15–17) and the conventional finite difference discretisations (20–22). Observe that for each stencil width, both the holistic and the conventional discretisations are consistent to the same order in grid spacing $h$. However, the holistic discretisations have fewer error terms than their corresponding conventional finite difference approximation. The holistic discretisations better model the nonlinear terms through the resolution of subgrid scale structures.

## 4 Holistic models accurately give steady states

The relevance of our holistic models is rigorously supported by centre manifold theory for sufficiently small parameters $\gamma$ and $\alpha$. However, the holistic models must be evaluated at coupling parameter $\gamma = 1$ to model the Kuramoto–Sivashinsky dynamics. The important question is: Does evaluating the holistic models at $\gamma = 1$ provide useful and accurate numerical models? Numerical experiments detailed in this and the next section provide strong support that it does.

In this section we explore the accuracy of the holistic models by constructing and comparing bifurcation diagrams of the various holistic discretisations to conventional explicit centered difference approximations and to the bifurcation diagrams presented by Jolly et al. [14] for various traditional Galerkin and nonlinear Galerkin approximations.

We restrict exploration to solutions that are both $2\pi$ periodic and odd: thus

$$u(x, t) = u(x + 2\pi, t) \quad \text{and} \quad u(x, t) = -u(2\pi - x, t). \quad (25)$$

We also restrict the nonlinearity parameter to the range $0 \leq \alpha \leq 70$. These restrictions are to compare our results to those of Jolly et al. [14] for approx-
Holistic models accurately give steady states

Figure 6: Accurate bifurcation diagram $0 \leq \alpha \leq 70$ for the Kuramoto–Sivashinsky equation, using a sixth order centered difference approximation with 48 points on the interval $[0, \pi]$. A signed $L^2$ norm is plotted against $\alpha$.

Such bifurcation diagrams usefully summarise qualitative and quantitative information for a large range of the nonlinearity parameter $\alpha$. We use the software package XPPAUT [8], which incorporates the continuation software AUTO [7], to calculate the bifurcation information. The information is then filtered through a function written in MATLAB to draw the bifurcation diagram. The input to XPPAUT is a text .ode file describing the set of ODEs. Because the holistic models contain a large number of terms the .ode files are generated automatically using REDUCE and MATLAB, see [19] for more details.
4 Holistic models accurately give steady states

4.1 The reference bifurcation diagram

Here we introduce accurate solutions for the steady states of the Kuramoto–Sivashinsky PDE (1) over the range $0 \leq \alpha \leq 70$ as summarised in the bifurcation diagram of Figure 6. The sixth order centered difference approximation (22) with 48 grid points on $[0, \pi]$ provides these accurate solutions. These provide the reference for the approximations on coarse grids, and serve to also introduce the conventions we adopt in bifurcation diagrams.

All the bifurcation diagrams plot a signed solution norm versus the nonlinearity parameter $\alpha$. Incorporating the sign is different to the plots of Jolly et al. [14] but empowers us to investigate more detail by separating positive and negative branches—stability differs along these branches. For example, Figure 6 shows that the negative bimodal branch is stable for $16.140 < \alpha < 22.556$, whereas the positive bimodal branch is unstable. The solution norm is signed corresponding to the sign of the first grid value, $u_1 = u(x_1)$. The blue curves are branches of stable fixed points and the red curves are branches of unstable fixed points. The open squares denote pitchfork bifurcations and the black squares denote Hopf bifurcations.

The labeling scheme used in Figure 6 follows that of Jolly et al. [14] and Scovel [31] with the addition of a plus or minus sign depending upon the sign of $u_1$. For example, the secondary bifurcation on the negative bimodal branch is labeled $R_2b_1$—from the labeling scheme of Scovel with the addition of the $-$ sign because it occurs on the negative branch. Figure 6 appears to show several discontinuities. For example, the positive unimodal branch ends at approximately $\alpha = 12$. This apparent discontinuity arises due to the convention adopted here of taking the sign of $u_1$ to sign the norm: actually there is a continuous transformation as the positive unimodal branch and the negative unimodal branch transform into the negative bimodal branch. It is straightforward to sign the branch near the trivial solution, but away from the trivial solution the distinction between positive and negative may be ambiguous and occasionally leads to jumps in the bifurcation diagram.

4.2 Holistic models are accurate on coarse grids

We investigate the reproduction of the bifurcation diagram, Figure 6, of the Kuramoto–Sivashinsky dynamics using coarse grids on the interval $[0, \pi]$ by both the holistic and centred difference discretisations. Bifurcation diagrams are analogous to skeletons for the dynamics: dynamically evolving solutions fit
that the holistic discretisations such as (15–17) provide reasonable solutions for significantly higher nonlinearity $\alpha$ than do the centred difference discretisations (20–22). We discuss bifurcation diagrams for $0 < \alpha < 70$.

4.2.1 Bifurcation diagrams show success

Now turn to the bifurcation diagram to obtain a more comprehensive view. We see the holistic model has good bifurcation diagrams on a coarse grid of 8 elements.

Figure 7 shows a side by side comparison of the holistic model with errors $O(\gamma^5, \alpha^2)$ with 8 elements on $[0, \pi]$ and the sixth order centered difference approximation with 8 grid points on $[0, \pi]$. These approximations are both 9 point stencil approximations. Plotted in grey, but without any stability information, is the accurate bifurcation diagram. The signed $L_2$ norms for the bifurcation diagrams on the coarse grid of 8 elements are adjusted by a factor of $\sqrt{6}$ to allow comparison to the accurate bifurcation diagram constructed with 48 grid points on $[0, \pi]$. When comparing bifurcation diagrams of different grid resolutions, the signed $L_2$ norms are adjusted this way to provide a consistent reference. Figure 7a shows the $O(\gamma^5, \alpha^2)$ holistic model gives good agreement with the accurate bifurcation diagram for $\alpha < 40$ and qualitatively reproduces around the steady states of a bifurcation diagram. Reproducing the ‘skeleton’ of the bifurcation diagram is crucial to accurate modelling.

Figure 7: Bifurcation diagrams for coarse grid approximations with 8 elements on $[0, \pi]$ for (a) holistic model (17), $O(\gamma^5, \alpha^2)$, (b) centered difference sixth order (22).
Table 2: \( \alpha \) values at which bifurcation points occur for the various coarse grid approximations; * denotes bifurcation point identified as fold point.

<table>
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<tr>
<th>Approximation</th>
<th>( R_2 b_1 )</th>
<th>( R_2 b_2 )</th>
<th>( R_2 b_3 )</th>
<th>( R_2 b_4 )</th>
<th>( R_3 t_1 )</th>
<th>( R_3 t_2 )</th>
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<td>44.70</td>
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<td>4th order ( (21) )</td>
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<td>35.98</td>
<td>48.62</td>
<td>63.11</td>
<td>62.98</td>
</tr>
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</table>

most of the bifurcation picture for \( 40 < \alpha < 70 \). The \( O(\gamma^5, \alpha^2) \) holistic model does not detect the bifurcation points \( R_3 t_2 \pm \) on this coarse grid and the bifurcation points \( R_3 t_1 \pm \) are incorrectly identified as fold points. However, the \( O(\gamma^5, \alpha^2) \) holistic model finds all of the other bifurcation points in this range of nonlinearity \( \alpha \). Figure 7b shows the sixth order centered difference approximation gives good agreement with the accurate bifurcation diagram only for \( \alpha < 20 \) and qualitatively reproduces the bifurcation diagram for \( 20 < \alpha < 40 \). The sixth order centered difference approximation performs poorly for \( \alpha > 40 \). Table 2 lists the values of \( \alpha \) at which the bifurcation points occur and confirms the \( O(\gamma^5, \alpha^2) \) holistic model performs more accurately than the sixth order centered difference approximation on this coarse grid of 8 elements.

MacKenzie [19] also showed how the holistic model reproduces more of the bifurcation diagram than the sixth order centered difference approximation even
Holistic models accurately give steady states

Figure 8: Bifurcation diagrams for the holistic models with 8 elements on the interval $[0, \pi]$ up to and including the $\mathcal{O}(\gamma^5, \alpha^4)$ holistic model.

We also investigate various holistic models for the Kuramoto–Sivashinsky PDE by comparing bifurcation diagrams of holistic models of higher orders. We examine bifurcation diagrams for holistic models with errors $\mathcal{O}(\gamma^p, \alpha^q)$, for $3 \leq p \leq 5$ and $2 \leq q \leq 4$, and find that retaining terms of higher order in coupling parameter $\gamma$, corresponding to wider stencil approximations, gives much greater improvement in accuracy than retaining terms of higher order in the nonlinearity parameter $\alpha$.

Figure 8 shows the bifurcation diagrams for the holistic models up to and including the $\mathcal{O}(\gamma^5, \alpha^4)$ holistic model. Surveying across the columns of Figure 8 see the bifurcation diagrams for holistic models of increasing order of coupling parameter $\gamma$, corresponding to approximations of increasing stencil width. For
example, the top row of Figure 8 shows the bifurcation diagrams for the holistic models (15), (16) and (17) respectively. Lower rows of Figure 8 display the bifurcation diagrams for increasing orders of the nonlinearity parameter $\alpha$. Figure 8 illustrates the improvement in accuracy of the higher order holistic models. Note first the dramatic improvement in accuracy gained by moving from left to right across Figure 8, corresponding to approximations of higher orders in the coupling parameter $\gamma$.

Second, less improvement is gained by moving from top to bottom of Figure 8, corresponding to approximations of higher order in the nonlinearity parameter $\alpha$. There are some peculiarities about this series of bifurcation pictures for holistic models of increasing order in $\alpha$. For the 5 point stencil approximations displayed in the left column of Figures 8, higher orders in $\alpha$ appear to gain some improvement. In particular Figures 8d,g show the $O(\gamma^3, \alpha^3)$ and $O(\gamma^3, \alpha^4)$ holistic models reproduce the unstable trimodal branches that were missing from the $O(\gamma^3, \alpha^2)$ bifurcation diagram shown in Figure 8a. However, for the 7 point stencil approximations displayed in the second column of Figure 8, holistic models of higher orders in $\alpha$ lose some features of the Kuramoto–Sivashinsky PDE. The correct behaviour of the unstable trimodal and quadrimal branches is reproduced for the $O(\gamma^4, \alpha^2)$ model shown in Figure 8b, but not reproduced for the higher order $O(\gamma^4, \alpha^3)$ and $O(\gamma^4, \alpha^4)$ models shown in Figures 8e,h respectively. For the 9 point stencil approximations, displayed in the third column of Figures 8, the $O(\gamma^5, \alpha^2)$ holistic model shown in Figure 8c, reproduces the unstable trimodal branch whereas the higher order $O(\gamma^5, \alpha^3)$ model shown in Figure 8f, does not reproduce the unstable trimodal branch. These peculiarities suggest that while we have observed excellent performance of the holistic models constructed with the non-local IBCs on coarse grids, it may be possible that modifications could be made to the non-local IBCs such that higher order approximations in the nonlinear parameter are improved. Further research will explore such possible modifications.

### 4.2.2 Holistic models outperform centered differences

Section 4.2.1 shows that the performance of the $O(\gamma^5, \alpha^2)$ holistic model (17) constructed with non-local IBCs is far superior to the explicit sixth order centered difference approximation (22). To complete the comparison of holistic models to explicit centered difference schemes, we compare the $O(\gamma^3, \alpha^2)$ (15) and $O(\gamma^4, \alpha^2)$ (16) holistic models to the second order (20) and fourth order (21) centered difference approximations; these are 5 point and 7 point discretisations respectively.
Holistic models accurately give steady states

Figure 9: Bifurcation diagrams for (a) $O(\gamma^3, \alpha^2)$ holistic model, (b) second order centered difference, (c) $O(\gamma^4, \alpha^2)$ holistic model and (d) fourth order centered difference all with 8 elements on the interval $[0, \pi]$

The first row of Figure 9 is a side by side comparison of the $O(\gamma^3, \alpha^2)$ holistic model and the second order centered difference approximation with 8 elements on $[0, \pi]$. The second row of Figure 9 is a side by side comparison of the $O(\gamma^4, \alpha^2)$ holistic model and the fourth order centered difference approximation on the same coarse grid. The accurate bifurcation diagram is plotted in grey without any stability information.

Although comparing Figures 9b,d shows some improvement is gained by taking higher order centered difference approximations, this improvement is not as pronounced as for the holistic models on this coarse grid as shown in Figures 9a,c. Both the second order and fourth order centered difference approximations fail to reproduce the correct behaviour of the unstable trimodal and
4 Holistic models accurately give steady states

Figure 10: Bifurcation diagrams for the holistic models with 12 elements on the interval $[0, \pi]$. Compare with Figure 8 with 8 elements.

quadrimodal branches. In contrast, even the 5 point stencil $O(\gamma^3, \alpha^2)$ holistic approximation qualitatively reproduces the trimodal and quadrimodal branches on the same coarse grid. The values at which the bifurcation points occur are listed in Table 2 and confirm these holistic models outperform the centered difference approximations on this coarse grid of 8 elements on $[0, \pi]$.

4.2.3 Grid refinement improves accuracy

Since the equivalent PDE’s (24) for our holistic models are of $O(h^2)$, $O(h^4)$ and $O(h^6)$ consistency respectively, see Table 1, grid refinement should result in improved accuracy.

Figure 10 shows the bifurcation diagrams of the holistic models up to and
including the $O(\gamma^4, \alpha^3)$ model on a finer grid of 12 elements on $[0, \pi]$. Compare Figure 10 with Figure 8 to confirm the improved accuracy for the holistic models on this refined grid. Table 2 also shows the bifurcation points are more accurately reproduced for the holistic models on this refined grid.

## 4.3 Comparison to Galerkin approximations

Here we investigate the traditional Galerkin and non-linear Galerkin approximations [14] for the Kuramoto–Sivashinsky equation (1) with the periodic and odd conditions (25). We find the holistic models compare well with the Galerkin methods. While the Galerkin methods are of superior accuracy for solving the Kuramoto–Sivashinsky PDE (1) with periodic boundary conditions, because of their global nature they lack the flexibility of the local nature of the holistic models. Although not explored here, this local nature of the holistic models empowers its use with physical boundary conditions [27] other than periodic.

Galerkin methods seek solutions in the form which is dominantly the superposition of $m$ periodic, global modes:

$$u(x, t) = \sum_{k=1}^{m} b_k(t) \sin(kx).$$  \hfill (26)

### The $m$-mode traditional Galerkin approximation

is

$$\frac{db_k}{dt} \approx (-4k^4 + \alpha k^2) b_k - \alpha \beta^m_k, \quad 1 \leq k \leq m,$$  \hfill (27)

where

$$\beta^m_k(b_1, \ldots, b_m) = \frac{1}{2} \sum_{j=1}^{m} j b_j \left[ b_{k+j} + \text{sign}(k-j)b_{|k-j|} \right].$$  \hfill (28)

### The $m$-mode first iterate nonlinear Galerkin approximation

is based upon the adiabatic approximation (30) for higher wavenumber modes $k = m+1 : 2m$, namely

$$\frac{db_k}{dt} \approx (-4k^4 + \alpha k^2) b_k - \alpha \beta^m_k(b_1, \ldots, b_m, \phi_{m+1}, \ldots, \phi_{2m}),$$  \hfill (29)

for $1 \leq k \leq m$, where

$$\phi_j = -\frac{\alpha}{4j^4} \beta^m_j(b_1, \ldots, b_m, 0, \ldots, 0),$$  \hfill (30)
Holistic models accurately give steady states

Figure 11: Bifurcation diagrams for (a) 3 mode, (b) 4 mode, (c) 6 mode and (d) 8 mode traditional Galerkin approximations on \([0, \pi]\).

for \(m + 1 \leq j \leq 2m\) and \(\beta_{j}^{2m}\) is given by (28).

Obtain higher order nonlinear Galerkin approximations \([22]\) through recognising time derivatives of these and even higher wave number modes. We do not explore such higher order Galerkin approximations.

Now examine the bifurcation diagrams of the two Galerkin approximations \((26–30)\) for \(0 \leq \alpha \leq 70\) and compare with the bifurcation diagrams of the holistic models on coarse grids, presented in \(\S 4.2\). Figure 11 shows the bifurcation diagrams for the 3 mode, 4 mode, 6 mode and 8 mode traditional Galerkin approximations on \([0, \pi]\). See that at least 4 modes are needed to qualitatively reproduce the behaviour of the stable bimodal branch. The \(\mathcal{O}(\gamma^5, \alpha^2)\) holistic model with 8 elements from Figure 7a and the 8 mode traditional Galerkin
Holistic models accurately give steady states

Figure 12: Bifurcation diagrams for (a) 3 mode, (b) 4 mode, (c) 6 mode and (d) 8 mode first iterate nonlinear Galerkin approximations on $[0, \pi]$. 

approximation qualitatively model most steady state dynamics. However, the 8 mode traditional Galerkin approximation is more accurate.

Figure 12 shows the bifurcation diagrams for the 3 mode, 4 mode, 6 mode and 8 mode first iterate nonlinear Galerkin approximations (29) on $[0, \pi]$. See impressive accuracy for the low mode first iterate nonlinear Galerkin approximations. The 6 mode nonlinear Galerkin approximation reproduces all of the steady state dynamics for the range $0 \leq \alpha \leq 70$. There is no discernible difference between the bifurcation diagram of the 8 mode nonlinear Galerkin approximation and the accurate bifurcation diagram for this range of $\alpha$. Table 3 lists the values of nonlinearity parameter $\alpha$ at which bifurcation points occur for the coarse grid holistic models and the Galerkin approximations [14]. The low mode first iterate nonlinear Galerkin approximations are impressively
Table 3: $\alpha$ values at which bifurcation points occur for the various coarse grid holistic models and low mode Galerkin approximations (‘k-m’ denotes k mode Galerkin).

<table>
<thead>
<tr>
<th>Approximation</th>
<th>$R_2 b_1$</th>
<th>$R_2 b_2$</th>
<th>$R_2 b_3$</th>
<th>$R_2 b_4$</th>
<th>$R_3 t_1$</th>
<th>$R_3 t_2$</th>
<th>$R_4 b_1$</th>
<th>$R_4 q_1$</th>
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<td></td>
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<td></td>
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<tr>
<td>Holistic 8 elements</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$O(\gamma^3, \alpha^2)$ (15)</td>
<td>14.64</td>
<td>20.36</td>
<td>39.34</td>
<td>44.96</td>
<td>29.28*</td>
<td>—</td>
<td>45.28</td>
<td>44.87</td>
</tr>
<tr>
<td>$O(\gamma^3, \alpha^3)$</td>
<td>14.65</td>
<td>20.52</td>
<td>39.66</td>
<td>45.16</td>
<td>29.33*</td>
<td>—</td>
<td>45.47</td>
<td>44.96</td>
</tr>
<tr>
<td>$O(\gamma^3, \alpha^4)$</td>
<td>14.65</td>
<td>20.53</td>
<td>39.72</td>
<td>45.21</td>
<td>29.33*</td>
<td>—</td>
<td>45.51</td>
<td>44.97</td>
</tr>
<tr>
<td>$O(\gamma^4, \alpha^2)$ (16)</td>
<td>16.00</td>
<td>22.56</td>
<td>48.62</td>
<td>57.38</td>
<td>34.73*</td>
<td>—</td>
<td>57.89</td>
<td>57.49</td>
</tr>
<tr>
<td>$O(\gamma^4, \alpha^3)$</td>
<td>16.00</td>
<td>22.56</td>
<td>48.25</td>
<td>56.84</td>
<td>34.73*</td>
<td>—</td>
<td>57.45</td>
<td>57.28</td>
</tr>
<tr>
<td>$O(\gamma^4, \alpha^4)$</td>
<td>16.00</td>
<td>22.57</td>
<td>48.10</td>
<td>56.63</td>
<td>34.73*</td>
<td>—</td>
<td>57.30</td>
<td>57.21</td>
</tr>
<tr>
<td>$O(\gamma^5, \alpha^2)$ (17)</td>
<td>16.13</td>
<td>22.72</td>
<td>51.54</td>
<td>61.54</td>
<td>35.89*</td>
<td>—</td>
<td>62.20</td>
<td>61.78</td>
</tr>
<tr>
<td>$O(\gamma^5, \alpha^3)$</td>
<td>16.13</td>
<td>22.73</td>
<td>51.53</td>
<td>61.37</td>
<td>35.91*</td>
<td>—</td>
<td>62.04</td>
<td>61.70</td>
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<tr>
<td>$O(\gamma^5, \alpha^4)$</td>
<td>16.13</td>
<td>22.73</td>
<td>51.60</td>
<td>61.38</td>
<td>35.91*</td>
<td>—</td>
<td>62.02</td>
<td>61.69</td>
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<tr>
<td>Holistic 12 elements</td>
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<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$O(\gamma^3, \alpha^2)$ (15)</td>
<td>15.45</td>
<td>21.67</td>
<td>45.96</td>
<td>53.94</td>
<td>32.86</td>
<td>45.98</td>
<td>54.49</td>
<td>54.17</td>
</tr>
<tr>
<td>$O(\gamma^3, \alpha^3)$</td>
<td>15.45</td>
<td>21.69</td>
<td>46.05</td>
<td>54.00</td>
<td>32.87</td>
<td>46.33</td>
<td>54.55</td>
<td>54.20</td>
</tr>
<tr>
<td>$O(\gamma^4, \alpha^2)$ (16)</td>
<td>16.11</td>
<td>22.62</td>
<td>51.93</td>
<td>62.10</td>
<td>35.90</td>
<td>50.92</td>
<td>62.83</td>
<td>62.52</td>
</tr>
<tr>
<td>$O(\gamma^4, \alpha^3)$</td>
<td>16.11</td>
<td>22.62</td>
<td>51.94</td>
<td>62.10</td>
<td>35.90</td>
<td>50.94</td>
<td>62.83</td>
<td>62.52</td>
</tr>
<tr>
<td>Galerkin [14]</td>
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<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3-m Euler–Galerkin</td>
<td>16.10</td>
<td>20.59</td>
<td>246.14</td>
<td>—</td>
<td>36.21</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>3-m Pseudo-stdy II</td>
<td>16.13</td>
<td>21.93</td>
<td>102.90</td>
<td>—</td>
<td>36.21</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>3-m Pseudo-stdy</td>
<td>16.13</td>
<td>22.01</td>
<td>93.91</td>
<td>—</td>
<td>36.24</td>
<td>63.91</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>12-m traditional</td>
<td>16.14</td>
<td>22.56</td>
<td>52.89</td>
<td>63.74</td>
<td>36.23</td>
<td>50.91</td>
<td>64.56</td>
<td>64.28</td>
</tr>
<tr>
<td>6-m traditional</td>
<td>16.14</td>
<td>22.55</td>
<td>52.72</td>
<td>63.28</td>
<td>36.23</td>
<td>46.85</td>
<td>64.00</td>
<td>64.00</td>
</tr>
<tr>
<td>3-m traditional</td>
<td>16.14</td>
<td>16.00</td>
<td>16.0</td>
<td>16.0</td>
<td>36.00</td>
<td>36.0</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

This evidence suggests that the holistic models are competitive with traditional Galerkin approximations, but that nonlinear Galerkin models are significantly better. However, recall that the holistic models are based upon analysis of local dynamics and thus we expect them to be more flexibly useful in applications than the global methods of these Galerkin approximations which not only rely on global eigenfunctions being known, here the sine functions, but also knowing closed form expressions for nonlinear combinations of the eigenfunctions. Furthermore, even when the nonlinear combinations of the eigenfunctions are known, the operation count of the nonlinear Galerkin method is high. For example, evaluating the time derivatives in (29) costs roughly $3m^2$ operations. Being quadratic in the number $m$ of modes, this evaluation is not scalable in...
the size of the domain. However, a holistic model with $m$ elements to some order $O(\gamma^p, \alpha^q)$ will evaluate all necessary time derivatives in a time proportional to $m$ and is thus scalable. True, the constant of proportionality may be rather large for any given order of truncation due to the modelling of the subgrid and interelement interactions. Nonetheless, holistic discretisation is scalable whereas Galerkin modelling is not.

**4.4 Coarse grids allow large time steps**

A major benefit of accurate models on coarse grids is that larger time steps are possible while maintaining numerical stability. §4.2 shows the remarkable accuracy of the $O(\gamma^5, \alpha^2)$ holistic model (17) on a coarse grid of 8 elements. Here we investigate the maximum stable time step for explicit Runge–Kutta time integration on various holistic models—implicit integration schemes are not considered here.

In particular, we compare approximations of similar accuracy but different grid resolutions to demonstrate the superior performance of the holistic models. MacKenzie [19] showed that the $O(\gamma^5, \alpha^2)$ holistic model (15) on 8 elements is of similar accuracy to the 16 point second order centered difference approximation (20). Thus we compare the computability of these two schemes.

Numerical experiments used the fourth order Runge–Kutta scheme to estimate the maximum stable time step for different holistic models and centered difference approximations at various values of nonlinearity parameter $\alpha$. Table 4 lists the approximate maximum time steps that maintain numerical stability along both the negative unimodal branch at $\alpha = 10$, and the negative bimodal branch at $\alpha = 20$ and $\alpha = 30$. For the $O(\gamma^5, \alpha^2)$ holistic model with 8 elements, the maximum time step maintaining numerical stability is approximately 10 times larger than the corresponding time step for the second order centered difference approximation with 16 grid points. The $O(\gamma^5, \alpha^2)$ holistic model requires approximately three times the number of floating point operations per grid value at each time step compared to the second order centered difference approximation. However, on a coarse grid of 16 points the second order centered difference approximation must be applied at twice as many grid points. Thus the $O(\gamma^5, \alpha^2)$ holistic model can be integrated an order of magnitude faster than the second order centered difference approximation while maintaining similar accuracy.

Note: Table 4 shows that the higher order terms in the nonlinearity $\alpha$, generated by the holistic method, do not reduce numerical stability.
Table 4: Approximate maximum time steps for stability of fourth order Runge–Kutta scheme.

<table>
<thead>
<tr>
<th>Approximation</th>
<th>( \alpha = 10 )</th>
<th>( \alpha = 20 )</th>
<th>( \alpha = 30 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Holistic 8 elements</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( O(\gamma^3, \alpha^2) ) (15)</td>
<td>.0011</td>
<td>.0014</td>
<td>.0017</td>
</tr>
<tr>
<td>( O(\gamma^3, \alpha^3) )</td>
<td>.0011</td>
<td>.0014</td>
<td>.0017</td>
</tr>
<tr>
<td>( O(\gamma^3, \alpha^4) )</td>
<td>.0011</td>
<td>.0014</td>
<td>.0017</td>
</tr>
<tr>
<td>( O(\gamma^4, \alpha^2) ) (16)</td>
<td>.0006</td>
<td>.0007</td>
<td>.0008</td>
</tr>
<tr>
<td>( O(\gamma^4, \alpha^3) )</td>
<td>.0006</td>
<td>.0007</td>
<td>.0008</td>
</tr>
<tr>
<td>( O(\gamma^4, \alpha^4) )</td>
<td>.0005</td>
<td>.0005</td>
<td>.0006</td>
</tr>
<tr>
<td>( O(\gamma^5, \alpha^2) ) (17)</td>
<td>.0005</td>
<td>.0005</td>
<td>.0006</td>
</tr>
<tr>
<td>( O(\gamma^5, \alpha^3) )</td>
<td>.0005</td>
<td>.0005</td>
<td>.0006</td>
</tr>
<tr>
<td>Centered 8 points</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2nd order (20)</td>
<td>.0011</td>
<td>.0012</td>
<td>—</td>
</tr>
<tr>
<td>4th order (21)</td>
<td>.0006</td>
<td>.0007</td>
<td>.0008</td>
</tr>
<tr>
<td>6th order (22)</td>
<td>.0005</td>
<td>.0005</td>
<td>.0006</td>
</tr>
<tr>
<td>Centered 16 points</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2nd order (20)</td>
<td>.00006</td>
<td>.00006</td>
<td>.00006</td>
</tr>
</tbody>
</table>

Stencils holistic approximations reduce the maximum stable time step somewhat, but so do the wider stencil conventional centered difference approximations. Thus, bear in mind that we need to balance the accuracy gained by using higher order approximation in \( \gamma \), that is, wider stencil approximations, with the reduction in numerical stability and the increase in computation per grid value.

5 Holistic models are accurate for time dependent phenomena

The Kuramoto–Sivashinsky equation (1) has rich dynamics [16, 14, 15, 31, 5, 12, 6, 2]. Having established the excellent performance of the holistic models in reproducing the steady states of the Kuramoto–Sivashinsky PDE in Section 4, we now investigate the holistic models performance at reproducing time dependent phenomena. The Kuramoto–Sivashinsky PDE exhibits complex time dependent behaviour such as limit cycles, period doubling and spatio-temporal chaos. This provides us with an example to explore the holistic approach to modelling time dependent phenomena with relatively coarse discretisations.
We restrict attention to $2\pi$ periodic solutions,

$$u(x, t) = u(x + 2\pi, t).$$  \hfill (31)

Initially we restrict further to solutions with odd symmetry, as in the previous section, which exhibit, see Figure 6, Hopf bifurcations to limit cycle solutions, and subsequent period doubling bifurcations apparently leading to low-dimensional chaos \cite{Kuroshige1, Kuroshige2, Kuroshige3}. In §5.1 we examine the dynamics of the holistic models on coarse grids through the eigenvalues of the models near the steady states. For example, we see that the $O(\gamma^5, \alpha^2)$ holistic model reproduces much of the eigenvalue information for $0 \leq \alpha \leq 70$ on a coarse grid of 8 elements. In §5.2 we explore the bifurcation diagrams near the first Hopf bifurcation and capture the stable limit cycles and period doubling sequence. The holistic models more accurately model the dynamics than centered difference approximations of equal stencil width. Subsequently we just require spatial periodicity whence stable travelling wave appear followed by, at higher values of nonlinearity parameter $\alpha$, more complex spatio-temporal chaos as investigated by Holmes, Lumley & Berkooz \cite{Holmes} and Dankowicz et al. \cite{Dankowicz}. In §5.3 we find the holistic discretisations more accurately model the amplitude and wave speed of travelling wave solutions, and predict better space time plots and time averaged power spectra, than corresponding the centered difference approximations.

### 5.1 Dynamics near steady states are reproduced

Consider the eigenvalues of the Kuramoto–Sivashinsky PDE (1) linearised about the steady states and restricted to odd symmetry. Accurate modelling of the eigenvalues near the steady states is a necessary condition for the accurate modelling of the dynamics.

**Compare eigenvalues along the bimodal branch** Consider the real part of the four largest (least negative real part) eigenvalues for low order holistic models and compare to explicit centered difference approximations on a coarse grid of 8 elements on $[0, \pi]$. Figure 13 shows the four largest eigenvalues for the $O(\gamma^3, \alpha^2)$ \eqref{gamma3alpha2}, $O(\gamma^4, \alpha^2)$ \eqref{gamma4alpha2} and $O(\gamma^5, \alpha^2)$ \eqref{gamma5alpha2} holistic models in green and the accurate solution in blue.\footnote{As in Section 4, a sixth order centered difference approximation with 48 grid points on $[0, \pi]$ provides the accurate reference for solutions.} Figure 13c, shows the four largest eigenvalues for the $O(\gamma^5, \alpha^2)$ holistic model closely matches the accurate solution over this range of nonlinearity parameter $\alpha$. 

Tony Roberts, November 22, 2006
Holistic models are accurate for time dependent phenomena

Figure 13: The four largest (least negative) eigenvalues along the stable bimodal branch for the (a) $O(\gamma^3, \alpha^2)$ (15), (b) $O(\gamma^4, \alpha^2)$ (16), (c) $O(\gamma^5, \alpha^2)$ (17) holistic models shown in green for 8 elements on $[0, \pi]$. Accurate eigenvalues are shown in blue.

Similarly, Figure 14 shows the four largest eigenvalues for the second order (20), fourth order (21) and sixth order (22) centered difference approximations in magenta on the same coarse grid. The centered difference approximations shown here are of equal stencil width to the corresponding holistic models in Figure 13. Figure 14a, shows the second order centered difference barely approximates the behaviour of the stable bimodal branch for $\alpha < 20$. Even the sixth order centered difference approximation, Figure 14c, is inferior to the $O(\gamma^4, \alpha^2)$ holistic model for $\alpha > 30$. This is despite the sixth order centered difference model having a wider stencil of 9 points compared to the 7 point stencil of the $O(\gamma^4, \alpha^2)$ holistic model. Figures 13 and 14 show the low order holistic models are superior to the corresponding centered difference approximations for reproducing the dynamics near the stable bimodal branch.

**Compare eigenvalues across the bifurcation diagram** Here we explore a new view of the earlier bifurcation diagrams that additionally depicts the real part of the 8 largest (least negative) eigenvalues by colour. Compare the eigenvalues of the $O(\gamma^5, \alpha^2)$ (17) holistic model, see Figure 15, on the coarse grid of 8 elements on $[0, \pi]$ to accurate ones for the Kuramoto–Sivashinsky PDE, see Figure 16, over the nonlinearity parameter $0 \leq \alpha \leq 70$. Colours code the magnitude of the real part of the eigenvalues according to the colour bar shown; the least negative eigenvalues are plotted above the more negative to give a small band of colour for each branch of steady states at each parameter value. Similarly to the bifurcation diagrams shown in Section 4, the open squares denote bifurcation points and the black squares denote Hopf bifurcations. Figure 15,
5 Holistic models are accurate for time dependent phenomena

Figure 14: The four largest eigenvalues along the stable bimodal branch for the (a) second order (20), (b) fourth order (21), (c) sixth order (22) centered difference approximations shown in magenta for 8 grid points on $[0, \pi]$. Accurate eigenvalues are shown in blue.

Figure 15: Bifurcation diagram of the $\mathcal{O}(\gamma^5, \alpha^2)$ holistic model (15) with 8 elements and odd symmetry on $[0, \pi]$, depicting the real parts of the 8 largest (least negative) eigenvalues colour coded according to the colour bar shown.
Figure 16: Bifurcation diagram of the accurate Kuramoto–Sivashinsky PDE, depicting the real parts of the 8 largest (least negative) eigenvalues, colour coded according to the colour bar shown.

when compared to Figure 16, shows that in addition to reproducing the stability of the accurate Kuramoto–Sivashinsky PDE for $0 \leq \alpha \leq 70$ as discussed in §4.2, the $O(\gamma^5, \alpha^2)$ holistic model reproduces well the eigenvalues for most of this range of nonlinearity parameter $\alpha$. This accurate modelling of the eigenvalues is evidence of accurate modelling of the Kuramoto–Sivashinsky dynamics, at least near the steady states.

### 5.2 Extend the Hopf bifurcations

Hopf bifurcations give rise to time periodic solutions (limit cycles). We explore the predictions of the various models to see how well they capture these strongly time dependent phenomena.

Here we investigate the bifurcation diagrams obtained by extending the first
Hopf bifurcation, at $\alpha = 30.345$, on the positive bimodal branch and the period doubling sequence that ensues. Trajectories in the period doubling sequence are reported and compared by MacKenzie [19]. As before, the holistic models outperform the corresponding centered difference approximations.

**Investigate the first Hopf bifurcation** $\text{HB}_1$ with a coarse grid of 8 elements on $[0, \pi]$. Figure 17 shows the bifurcation diagrams of the low order holistic models and the accurate bifurcation diagram near the first Hopf bifurcation. The stable limit cycles (light blue) that continue from this bifurcation point undertake a period doubling sequence commencing at a point labeled PD (yellow square). The pair of unstable limit cycles born at PD give rise to the period doubling sequence leading to chaos.

The accurate bifurcation diagram shown is identical to the bifurcation diagram for the same range of $\alpha$ produced by Jolly et al. [14]. Figure 17a, shows that even the lowest order $\mathcal{O}(\gamma^3, \alpha^2)$ (15) holistic model reproduces the the first Hopf bifurcation and finds the period doubling point on this coarse grid of 8 elements.\(^7\) In comparison, the corresponding second order centered difference approximation does not even have the first Hopf bifurcation, see Figure 9b.

Figure 17b,c, show that higher order holistic models accurately model the first Hopf bifurcation and the resulting stable and unstable limit cycles. The accuracy of the $\mathcal{O}(\gamma^5, \alpha^2)$ holistic model (17) for reproducing these periodic solutions of the Kuramoto–Sivashinsky PDE is remarkable on this coarse grid. Figure 18 shows the corresponding bifurcation diagrams for the fourth order and sixth order centered difference approximations with 8 grid points on $[0, \pi]$. Compare Figure 18 and Figure 17 to see that the sixth order centered difference approximation which has a nine point stencil does not perform as well as the $\mathcal{O}(\gamma^4, \alpha^2)$ holistic model (16) which has a 7 point stencil. Figure 17b,c, show that higher order holistic models more accurately model the first Hopf bifurcation and the resulting stable and unstable limit cycles. Table 5 shows the parameter values $\alpha$ for the Hopf bifurcations, $\text{HB}_1$, and the initial period doubling point PD: both the $\mathcal{O}(\gamma^4, \alpha^2)$ and $\mathcal{O}(\gamma^5, \alpha^2)$ holistic models are more accurate than the fourth order and sixth order centered difference approximations in reproducing the first Hopf bifurcation and the resulting period doubling point.

\(^7\)Figure 17a displays the bifurcation diagram for $25 \leq \alpha \leq 32$ compared to $30 \leq \alpha \leq 37$ for the other diagrams. Since the first Hopf bifurcation for the $\mathcal{O}(\gamma^3, \alpha^2)$ holistic model occurs at $\alpha = 25.595$ the bifurcation diagram is shifted to contain the important dynamics.
Table 5: Nonlinearity parameter $\alpha$ values for the first Hopf bifurcation point $\text{HB}_1$ and resulting period doubling point $\text{PD}$.

<table>
<thead>
<tr>
<th>Approximation</th>
<th>$\text{HB}_1$</th>
<th>$\text{PD}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Holistic 8 elements</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\mathcal{O}(\gamma^3, \alpha^2)$ (15)</td>
<td>25.60</td>
<td>27.22</td>
</tr>
<tr>
<td>$\mathcal{O}(\gamma^4, \alpha^2)$ (16)</td>
<td>30.04</td>
<td>32.03</td>
</tr>
<tr>
<td>$\mathcal{O}(\gamma^5, \alpha^2)$ (17)</td>
<td>30.66</td>
<td>32.95</td>
</tr>
<tr>
<td>Centered 8 points</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2nd order (20)</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>4th order (21)</td>
<td>27.91</td>
<td>29.57</td>
</tr>
<tr>
<td>6th order (22)</td>
<td>29.11</td>
<td>31.40</td>
</tr>
<tr>
<td>Accurate</td>
<td>30.35</td>
<td>32.97</td>
</tr>
</tbody>
</table>

5.3 Dynamics of periodic patterns without odd symmetry

Consider the Kuramoto–Sivashinsky PDE (1) with solutions that are spatially periodic (31)—we remove the requirement for odd symmetry. Consequently, we now explore travelling wave like solutions at low nonlinearity $\alpha$. Also we illustrate the spatio-temporal chaos that occurs at higher $\alpha$.

**Good performance for holistic models at low nonlinearity $\alpha$** Consider the holistic models of the Kuramoto–Sivashinsky PDE (1) and (31) for nonlinearity parameter $\alpha = 5$ and $\alpha = 10$ on coarse grids of 8 elements on $[0, 2\pi]$; that is, the element size is twice as big as many earlier solutions because the domain is twice as big. Figure 3 shows solutions obtained from the lowest order $\mathcal{O}(\gamma^3, \alpha^2)$ holistic model (15) for $\alpha = 5$ in green, the accurate solution in blue and the corresponding second order centered difference approximation (20) with 8 points on $[0, 2\pi]$, in magenta. The solutions are shown starting from the half-wave initial condition of $u(x, 0) = |\sin(x/2)|$. See the $\mathcal{O}(\gamma^3, \alpha^2)$ holistic model is superior to the second order centered difference approximation on this coarse grid. In particular, the amplitude of the evolving wave-like solution and the wave speed are more accurately reproduced by the $\mathcal{O}(\gamma^3, \alpha^2)$ holistic model for $\alpha = 5$.

Similarly, Figure 19 shows the solutions at the same times but for larger nonlinearity $\alpha = 10$. For this $\alpha$ the second order (20) and fourth order (21) centered difference approximations do not generate a wave-like solution at all.
However, the sixth order centered difference approximation (22) does produce the travelling wave-like solution shown in red. The $O(\gamma^3, \alpha^2)$ holistic model (green) is the least accurate on this coarse grid but it does reproduce a stable solution on this coarse grid for only a 5 point stencil approximation. The $O(\gamma^4, \alpha^2)$ holistic model (light green) more accurately models the amplitude of the wave compared to the sixth order centered difference approximation despite having a smaller stencil width. The $O(\gamma^5, \alpha^2)$ holistic model is the most accurate at reproducing the evolution of the stable wave-like solution for $\alpha = 10$ on this coarse grid of 8 elements.

**Good performance for more complex dynamics** For higher values of nonlinearity parameter $\alpha$ for which the Kuramoto–Sivashinsky pde exhibits more complex dynamics, including spatio-temporal chaos, we compare time averaged power spectra rather than particular travelling waves. Here we investigate the performance of the holistic models on coarse grids for $\alpha = 20$ and $50$ using the example of the $O(\gamma^5, \alpha^2)$ holistic model (17), and compare it with the sixth order centered difference approximation (22) as it is of equal stencil width. Further, we also compare the $O(\gamma^5, \alpha^2)$ holistic model on coarse grids to the second order centered difference approximations of similar accuracy. We find the $O(\gamma^5, \alpha^2)$ holistic model, but with approximately 1/3 of the grid points, has comparable accuracy to second order centered difference approximations.

Figure 20 shows space time plots of (a) the $O(\gamma^5, \alpha^2)$ holistic model (17), (b) the sixth order centered difference approximation (22), and (c) the accurate solution. The $O(\gamma^5, \alpha^2)$ holistic model reproduces much of the complex structure of the accurate solution for nonlinearity $\alpha = 20$ with 12 elements. Figure 20b, shows the sixth order centered difference approximation incorrectly finds a periodic solution after approximately $t = 0.2$. Similar behaviour occurs for nonlinear parameter $\alpha = 50$ with 24 elements [19]: the holistic discretisation accurately models the apparently chaotic dynamics; whereas the centred difference model incorrectly locks onto a periodic travelling wave.

Since the Kuramoto–Sivashinsky pde at nonlinearity parameter $\alpha = 20$ exhibits more complex time dependent behaviour than simple limit cycles, we compare time averaged power spectra, denoted here by $S(k)$ for wavenumber $k$. Figure 21a, shows a log-log plot of the time average power spectra of the $O(\gamma^5, \alpha^2)$ holistic model, the sixth order centered difference approximation

8The accurate solutions plotted in this section are computed using a sixth order centered difference approximation and 256 grid points on the interval $[0, 2\pi]$. This is sufficient grid resolution to capture the important dynamics of the Kuramoto–Sivashinsky pde for the values of $\alpha$ investigated here.
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on a coarse grid of 12 elements on $[0, 2\pi]$, and the accurate power spectrum. For this coarse grid of only 12 elements only 5 wavenumbers are relevant, as displayed. See that the $\mathcal{O}(\gamma^5, \alpha^2)$ holistic model is superior to the sixth order centered difference approximation on this coarse grid. Figure 21b, compares the time average power spectrum of the $\mathcal{O}(\gamma^5, \alpha^2)$ holistic model with 12 elements and the sixth order centered difference approximation with 16 grid points. The $\mathcal{O}(\gamma^5, \alpha^2)$ holonic model achieves similar accuracy on a coarser grid.

Figure 22a,b show the power spectra of the $\mathcal{O}(\gamma^5, \alpha^2)$ holistic model on a coarse grid of 12 elements and the second order centered difference approximation on the more refined grids of 24 and 36 points, respectively. A refined grid of 36 points is needed to achieve similar accuracy to the $\mathcal{O}(\gamma^5, \alpha^2)$ holistic model on a coarse grid of 12 elements on $[0, 2\pi]$. That is, through its subgrid scale modeling, the holistic model achieves similar accuracy with one-third the dimensionality.

This investigation of the $\mathcal{O}(\gamma^5, \alpha^2)$ holistic model on coarse grids for $\alpha = 20$ and that of MacKenzie [19] for nonlinearity $\alpha = 50$, shows it reproduces similar accuracy to the second order centered difference approximation on a coarse grid of approximately 1/3 the resolution, and similar accuracy to the sixth order centered difference approximation on grids of approximately 3/4 the resolution. MacKenzie [19] reports that even at $\alpha = 200$ the holistic model qualitatively well captures the dynamics of the Kuramoto–Sivashinsky PDE. This increased accuracy on coarse grids allows larger time steps for explicit time integration schemes, as discussed in \S 4.4.

6 Conclusion

Holistic discretisation [25] is straightforwardly extended to fourth order dissipative PDEs through the example of the Kuramoto–Sivashinsky equation [18]. We divide the domain into elements by introducing artificial internal boundary conditions (\S 2) which isolate the elements when $\gamma = 0$ but when $\gamma = 1$ they fully couple the elements to recover the Kuramoto–Sivashinsky dynamics. Then centre manifold theory supports the discretisation, see \S 2.2. The holistic models listed in \S 3 have a dual justification (\S 3.3): not only are they supported by centre manifold theory for finite element size $h$, the IBCs are specially crafted [26] so the models are also consistent with the Kuramoto–Sivashinsky equation as the grid spacing $h \rightarrow 0$.

No formal error bounds currently exist for the holistic method; the difficulty is that the models are based at $\gamma = 0$ but are evaluated at finite $\gamma = 1$. Instead
we present a detailed numerical investigation of the holistic models of the steady states (Section 4) and time dependent solutions (Section 5) of the Kuramoto–Sivashinsky on coarse grids.

We compared, in §4.4, the accuracy of different approximations in predicting steady states on different grid resolutions. The holistic $\mathcal{O}(\gamma^5, \alpha^2)$ approximation on a grid of 8 elements has similar accuracy to a second order centered difference approximation on a grid of 16 points. Consequently the holistic model allows a maximum time step which is an order of magnitude larger than that of the explicit centered difference approximation of similar accuracy, while maintaining numerical stability. The accuracy of the holistic approximations to the Kuramoto–Sivashinsky equation on coarse grids and subsequent improved performance justifies further application of the holistic method and future investigation of the approach.

Holistic models on coarse grids also model well time dependent phenomena of the Kuramoto–Sivashinsky PDE. In particular, in §5.1 we saw the holistic models more accurately model the eigenvalues near the steady states of the first form of the Kuramoto–Sivashinsky PDE compared to explicit centered difference approximations of equal stencil widths. The coarse grid holistic models also more accurately model the first Hopf bifurcation and the resulting period doubling sequence, see §5.2. Further, in comparison with explicit centered difference models, in §5.3, we saw good performance for higher values of the nonlinearity parameter $\alpha$ and more accurate predictions of time averaged power spectra: the $\mathcal{O}(\gamma^5, \alpha^2)$ holistic model achieves similar accuracy to the second order and sixth order centered difference approximations on approximately 1/3 and 3/4 of the grid resolutions respectively.

This good performance of the holistic models for accurately reproducing both the steady states and the time dependent phenomena of the Kuramoto–Sivashinsky PDE is good evidence that the holistic approach is a powerful method for discretising dissipative PDEs on coarse grids.

References


References


Figure 17: Bifurcation diagrams near the first Hopf bifurcation for (a) $\mathcal{O}(\gamma^3, \alpha^2)$ (15), (b) $\mathcal{O}(\gamma^4, \alpha^2)$ (16), (c) $\mathcal{O}(\gamma^5, \alpha^2)$ (17) holistic models with 8 elements on $[0, \pi]$ and (d) an accurate bifurcation diagram. Stable limit cycles are shown in light blue and unstable limit cycles are shown in orange.
Figure 18: Bifurcation diagrams near the first Hopf bifurcation for (a) fourth order \((21)\), (b) sixth order \((22)\) centered difference approximations with 8 grid points on \([0, \pi]\). Stable limit cycles are shown in light blue and unstable limit cycles are shown in orange.
Figure 19: $\alpha = 10$: wave-like solutions at times $t = 0, 0.2, 0.4, 0.6, 0.8, 1$ for the $O(\gamma^3, \alpha^2)$ (15), $O(\gamma^4, \alpha^2)$ (16) and $O(\gamma^5, \alpha^2)$ (17) holistic models shown in green, light green and light blue respectively and the sixth order centered difference approximation (22) shown in red on a coarse grid of 8 elements on $[0, 2\pi]$. The accurate solution is shown in blue.
Figure 20: $\alpha = 20$: space time plots for (a) the $O(\gamma^5, \alpha^2)$ holistic model (17) with 12 elements on $[0, 2\pi]$, (b) sixth order centered difference approximation (22) with 12 grid points on $[0, 2\pi]$ and (c) the accurate solution.
Figure 21: $\alpha = 20$: time averaged power spectra for the $O(\gamma^5, \alpha^2)$ holistic model (17) with 12 elements on $[0, 2\pi]$ shown in light blue, and the sixth order centered difference approximation (22) in red for (a) 12 grid points on $[0, 2\pi]$ and (b) 16 grid points on $[0, 2\pi]$. The accurate power spectrum is shown in blue.
Figure 22: $\alpha = 20$: time averaged power spectra for the $O(\gamma^5, \alpha^2)$ holistic model with 12 elements on $[0, 2\pi]$ shown in light blue, and the second order centered difference approximation in magenta for (a) 24 grid points on $[0, 2\pi]$ and (b) 36 grid points on $[0, 2\pi]$. The accurate spectrum is shown in blue.