# Regularization of the Backward–in–Time Kuramoto–Sivashinsky Equation

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## Abstract

We are interested in solution techniques for backward-in-time evolutionary PDE problems arising in fluid mechanics. In addition to their intrinsic interest, such techniques have applications in the recently proposed retrograde data assimilation. As our model system we consider the terminal value problem for the Kuramoto–Sivashinsky equation in a 1D periodic domain. Such backward problems are typical examples of ill–posed problem, where any disturbances are amplified exponentially during the backward march. Hence, regularization is required in order to solve such problem efficiently in practice. We consider regularization approaches in which the original ill–posed problem is approximated with a less ill–posed problem obtained by adding a regularization term to the original equation. While such techniques are relatively well–understood for simple linear problems, in this work we investigate them carefully in the nonlinear setting and report on some interesting universal behavior. In addition to considering regularization terms with fixed magnitudes, we also mention briefly a novel approach in which these magnitudes are adapted dynamically using simple concepts from the Control Theory.

# 1 Introduction

The motivation for investigating a *terminal* value problem for a dissipative partial differential equation (PDE) comes from the recently-proposed retrograde framework for data assimilation [5,18]. In the atmospheric sciences, data assimilation is used, for example, to generate initial conditions for future weather forecasts based on some past measurements [10]. Such problems are typically solved using methods of PDE-constrained optimization to determine an initial condition in the past, such that the ensuing system evolution best matches the available measurements. Using this initial condition determined in the past to integrate the system until the present time, one can obtain an initial condition for a future forecast. In the classical formulation of the variational data assimilation known as 4DVAR [10] one needs to solve the governing PDE system forward in time, and the adjoint system backward in time, both of which are well–posed [8]. On the other hand, in the proposed retrograde framework, one solves the PDE-constrained optimization problem using the *terminal* state as the control variable, and as a result one must solve the governing PDE system backward in time, and the adjoint system forward in time, both of which are now ill-posed problems. The present investigation seeks to assess how accurately such ill-posed problems can be solved when regularization is applied. In addition, the issue of a numerical solution of terminal value problems for dissipative PDEs is also one of an independent interest.

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The Kuramoto–Sivashinsky equation was proposed in [13] and [22] to model instabilities of flame fronts and is often used as a model for nonlinear evolutionary systems, because in sufficiently large domains its solutions are characterized by self–sustained chaotic and multiscale behavior. The initial value problem for the Kuramoto–Sivashinsky equation is given by

$$\frac{\partial u}{\partial \tau} + u \frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2} + \frac{\partial^4 u}{\partial x^4} = 0, \quad \tau \in [0, T] \quad x \in [0, L], \\
\frac{\partial^i u(\tau, 0)}{\partial x^i} = \frac{\partial^i u(\tau, L)}{\partial x^i}, \quad \tau \in [0, T], \quad i = 0, \dots, 3, \quad (1.1) \\
u(0, x) = \phi(x), \quad x \in [0, L],$$

where  $u : [0,T] \times [0,L] \to \mathbb{R}$  is the solution and  $\phi : [0,L] \to \mathbb{R}$  the initial condition. Our focus here will be entirely on the case of one-dimensional (1D) periodic domains [0, L]. While there exist some results concerning the behavior of the Kuramoto–Sivashinsky system in a bounded domain [6], this system is typically studied in the periodic setting. Such formulation will make it possible to use elementary methods of the Fourier analysis to justify the proposed regularization strategies. We expect that the performance of these regularization strategies would be similar for systems defined on bounded domains, however, their mathematical characterization would be somewhat less straightforward. We emphasize that form (1.1) is generic, in the sense that forms of the equation involving coefficients other then unity in front of different terms (see, e.g., [9]) may always be reduced to (1.1)via a suitable (nonlinear) change of variables. As shown in [17], the size of the domain L plays a role similar to the Reynolds number in hydrodynamics in that it determines the behavior of the solutions. For small values of L the zero solution is the only stable solution, while as L increases, a sequence of bifurcations leads to different families of nontrivial fixed-point, traveling wave and, eventually, chaotic solutions [9]. In this investigation we will be mainly interested in such turbulent solutions corresponding to large values of L.

In the present study we will use the following *terminal* value problem for the Kuramoto–Sivashinsky equation

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} + \frac{\partial^2 v}{\partial x^2} + \frac{\partial^4 v}{\partial x^4} = 0, \quad t \in [0, T] \quad x \in [0, L],$$

$$\frac{\partial^i v(t, 0)}{\partial x^i} = \frac{\partial^i v(t, L)}{\partial x^i}, \quad t \in [0, T], \quad i = 0, \dots, 3, \quad (1.2)$$

$$v(T, x) = \varphi(x), \quad x \in [0, L],$$

where  $v : [0, T] \times [0, L] \to \mathbb{R}$  is the solution and  $\varphi : [0, L] \to \mathbb{R}$  the terminal condition, as a model to investigate regularization of backward–in–time problems for a class of nonlinear evolutionary PDEs. The difference between (1.1) and (1.2) is that in the initial value problem the data is provided at t = 0, while in the terminal value problem the data is provided at t = T. Solution of initial value problem (1.1) exists for all square–integrable initial conditions  $\phi$ , however, as regards terminal value problem (1.2), it was proved in [12] that a solution only exists when  $\varphi$  is on the attractor of system (1.1). If  $\varphi$  is not on the attractor, solutions of (1.2) will blow up such that  $\|v(t)\|_{L_2}^2$  goes towards infinity faster than any exponential as t decreases from T to 0 [11]. In other words, the solution to the terminal value problem may not exist on [0, T], unless one makes sure that  $\varphi$  actually comes from a solution of initial value problem (1.1); only such terminal conditions for (1.1) will be considered in the present work. To clarify further the mathematical relation between initial–value and terminal–value problems (1.1) and (1.2), we can rewrite the latter using the change of variables  $\overline{t} = T - t$  as the following initial–value problem

$$\frac{\partial v}{\partial \bar{t}} - v \frac{\partial v}{\partial x} - \frac{\partial^2 v}{\partial x^2} - \frac{\partial^4 v}{\partial x^4} = 0, \qquad \bar{t} \in [0, T] \qquad x \in [0, L], 
\frac{\partial^i v(\bar{t}, 0)}{\partial x^i} = \frac{\partial^i v(\bar{t}, L)}{\partial x^i}, \qquad \bar{t} \in [0, T], \qquad i = 0, \dots, 3, \qquad (1.3) 
v(0, x) = \varphi(x), \qquad \qquad x \in [0, L],$$

where all the terms, except for the time-derivative term, have reversed signs as compared to (1.1).

While the classical case of an ill–posed backward–in–time system, the terminal value problem for the heat equation, is well understood [14], terminal value problems for nonlinear PDEs have not been the focus of much previous research. It is tempting to think that the presence of convective–type nonlinearities, such as the term  $v \frac{\partial v}{\partial x}$  in (1.2), could render the problem more regular by reducing the relative effects due to the ill–posed "parabolic" part. We emphasize, however, that this is only a conjecture based on observations of forward Kuramoto–Sivashinsky system (1.1), and we are not aware of any rigorous results to this effect. It is thus one of the goals of our paper to verify this conjecture by investigating how the performance of regularization strategies developed for backward–in–time linear parabolic problems is affected by such nonlinearities.

The structure of the paper is as follows: Section 2 discusses some properties of the Kuramoto–Sivashinsky system in Fourier space; Section 3 introduces the regularization methods that we use; Section 4 presents the computational results concerning the performance of these regularization methods; summary of the main results and final conclusions are deferred to Section 5.

# 2 Kuramoto–Sivashinsky Equation — a Fourier Space Perspective

The nature of the ill–posedness and the mechanism of the numerical blow–up will be particularly evident when regarded in the Fourier space representation. This perspective will also guide the choice of physically–motivated regularization strategies for backward problem (1.2). Representing  $u(\tau, x) = \sum_{\kappa \in \mathbb{K}} \hat{u}_{\kappa}(\tau) e^{i\kappa x}$ , where  $\hat{u}_{\kappa}(\tau) \in \mathbb{C}$  are the Fourier coefficients and the wavenumbers are defined as  $\kappa = k \frac{2\pi}{L}$ ,  $k \in \mathbb{Z}^+$  with  $\mathbb{K} = \{k\frac{2\pi}{L}, k \in \mathbb{Z}^+\}$ , system (1.1) can be expressed as

$$\frac{d\hat{u}_{\kappa}}{d\tau} = -\hat{w}_{\kappa} + \mathcal{A}(\kappa)\hat{u}_{\kappa}, \qquad \kappa \in \mathbb{K}, \qquad \tau \in [0, T]$$

$$\hat{u}_{\kappa}(0) = \hat{\phi}_{\kappa}, \qquad \kappa \in \mathbb{K},$$
(2.1)

where  $\mathcal{A}(\kappa) \triangleq \kappa^2 - \kappa^4$  is the operator corresponding to the linear part of the Kuramoto– Sivashinsky equation (" $\triangleq$ " means "equal to by definition"), and  $\hat{w}_{\kappa} = \left(\widehat{u\frac{\partial u}{\partial x}}\right)_{\kappa}$  is the Fourier transform of the nonlinear term [hats (^) will in general denote Fouriertransformed variables; we choose to use rescaled wavenumbers  $\kappa \in \mathbb{K}$  rather than  $k \in \mathbb{Z}$ , because they result in simpler expressions]. Since the solutions  $u(\tau, x)$  are real, we can restrict ourselves to nonnegative wavenumbers  $\kappa \ge 0$  only. The effect of the different terms in (2.1) can be phenomenologically interpreted as follows: the (unstable) second–order term injects energy at the intermediate wavenumbers  $\kappa$ , the (stable) fourth–order terms dissipates energy at the large wavenumbers, whereas the nonlinear term moves the energy between the different wavenumber ranges (as is evident from the identity  $\int_0^L u^2 \frac{\partial u}{\partial x} dx \equiv 0$ , on a periodic domain the nonlinear term does not produce energy). By examining the spectrum of the operator  $\mathcal{A}(\kappa)$  we note that the maximum energy injection occurs at the wavenumber  $\kappa_{max} = 1/\sqrt{2}$ , whereas  $\kappa_0 = 1$  marks the boundary between the energy injection and dissipation ranges. It is common to characterize solutions of evolutionary PDEs in Fourier space using the energy function defined as

$$E(\kappa) \triangleq \frac{1}{2} |\hat{u}_{\kappa}|^2, \quad \kappa \in \mathbb{K}.$$
 (2.2)

A typical instantaneous energy function for a solution of system (1.1) on a "turbulent" attractor is shown in Fig. 1. In addition to the features mentioned above, the plot of the energy function  $E(\kappa)$  reveals also a flat region for small wavenumbers indicative of a "white noise" behavior of the large–scale structures [7]. The region  $0.8 \leq \kappa \leq 1.25$  exhibits a power–law decay described approximately by  $\kappa^{-4}$  [24] which is why it is sometimes referred to as an "inertial range" similar to the scaling range observed in solutions of the Navier–Stokes system [17]. For high wavenumbers the energy function  $E(\kappa)$  tends towards zero exponentially fast which is consistent with the estimate [4]

$$|\hat{u}|_{\kappa} = O(e^{-\alpha\kappa}), \quad \text{for} \quad \kappa \to \infty,$$
 (2.3)

where  $\alpha > 0$ , applicable to infinitely differentiable functions periodic on [0, L].

## **3** Ill–Posedness and Regularization Techniques

Using the Fourier space representation of the solution  $v(t,x) = \sum_{\kappa \in \mathbb{K}} \hat{v}_{\kappa}(t) e^{i\kappa x}$ , terminal value problem (1.2) becomes

$$\frac{d\hat{v}_{\kappa}}{dt} = -\hat{w}_{\kappa} + \mathcal{A}(\kappa)\hat{v}_{\kappa}, \qquad \kappa \in \mathbb{K}, \qquad t \in [0, T]$$

$$\hat{v}_{\kappa}(T) = \hat{\varphi}_{\kappa}, \qquad \kappa \in \mathbb{K}.$$
(3.1)

We note that introducing the change of variables  $t = T - \tau$  one can convert (3.1) to an initial value problem in which, as compared to (2.1), the terms on the right-hand side (RHS) have reversed signs. This means that the role of the terms in the operator  $-\mathcal{A}(\kappa)$  will be interchanged: the fourth-order term will now act as an energy source, whereas the second-order term will act as an energy sink. As a result, during backward-in-time integration of (3.1) any perturbations, arising for instance from the truncation of the Fourier series representation of the terminal condition  $\varphi$ , are exponentially amplified. Indeed, numerical simulations confirm that the solution  $v(\tau)$  usually "blows up" (in the sense of numerical overflow errors in the finite-precision arithmetic) within a few time steps. This type of ill-posedness is generic in parabolic systems integrated backwards in time. It is typically studied in the context of the heat equation for which most of the regularization strategies



Fig. 1. The energy function  $E(\kappa)$  corresponding to a "turbulent" solution of initial value problem (1.1) with L = 154; the vertical line corresponds to  $\kappa_{max}$ ; for clarity, the wavenumbers  $\kappa$  are treated as a continuous variable.



(b)

Fig. 2. A qualitative sketch of the effect of regularization on the spectrum of the linear operator  $-\mathcal{A}(\kappa)$  for (a) hyperviscous regularization, and (b) pseudo–parabolic regularization: (solid line) spectrum of the linear operator  $-\mathcal{A}(\kappa)$ , (dotted lines) spectra of the regularized operators  $-\mathcal{B}_{\alpha}(\kappa)$  and  $-\mathcal{B}_{\beta}(\kappa)$ ; arrows represent the trends corresponding to the increase of the regularization parameter; for clarity, the wavenumbers  $\kappa$  are treated as a continuous variable.

were developed [14]. Given the qualitative similarity between the backward heat equation and the linear part of problem (1.2), we will proceed by adapting these methods to the problem at hand.

The idea of regularization is to replace the original ill–posed problem with another one that is more stable and in some suitably–defined sense close to the original problem. Evidently, in problem (3.1) the unboundedness of the operator  $-\mathcal{A}(\kappa)$  for  $\kappa \to \infty$  is the source of the ill–posedness. In the spirit of the "quasi–reversibility" approach developed by Lattés and Lions in [14], we propose to regularize this problem by replacing (3.1) with

$$\frac{d\hat{p}_{\kappa}}{dt} = -\hat{q}_{\kappa} + \mathcal{A}(\kappa)\hat{p}_{\kappa} + \mu(t)\mathcal{B}(\kappa)\hat{p}_{\kappa} 
\triangleq -\hat{q}_{\kappa} + \mathcal{A}_{\mu}(\kappa)\hat{p}_{\kappa}, \qquad \kappa \in \mathbb{K}, \quad t \in [0,T] \quad (3.2) 
\hat{p}_{\kappa}(T) = \hat{\varphi}_{\kappa}, \qquad \kappa \in \mathbb{K}.$$

where  $\hat{q}_{\kappa} = \left(p\frac{\partial p}{\partial x}\right)_{\kappa}$ ,  $\mu(t) \in \mathbb{R}^+$  is a small "regularization parameter" that in general may be a function of time  $\mu : [0,T] \to \mathbb{R}^+$ , and  $\mathcal{B}(\kappa)$  is a regularization operator chosen to "correct" the behavior of  $-\mathcal{A}(\kappa)$  for large  $\kappa$ . Two choices of the regularization operator  $\mathcal{B}(\kappa)$  will be discussed in Sections 3.1 and 3.2 below. Thus, for a given form of  $\mathcal{B}(\kappa)$ , the main challenge consists in choosing the regularization parameter  $\mu$ , so that the regularized solution  $p(t,x) = \sum_{\kappa \in \mathbb{K}} \hat{p}_{\kappa}(t)e^{i\kappa x}$  is stable and, at least for some time, close to the solution of original problem (3.1) in which no perturbation was allowed to appear. As we will see, these requirements are in fact contradictory, and the choice of  $\mu$  will have to represent a trade–off between them. In the case of linear problems, such optimal values of the regularization parameter this is not possible and one has to resort to numerical computations. For the most part we will consider *constant* values of the regularization parameter  $\mu(t) = \mu$ . We

will focus on two forms of the operator  $\mathcal{B}(\kappa)$  that will result in the so-called "hyperviscous" and "pseudo-parabolic" regularization. Other forms of regularization have also been considered in the literature, e.g., "hyperbolization" [2], variational techniques [15,16], convolution with a filter, Galerkin projection, etc., but they will not be addressed in the present study. We will instead briefly consider generalization of the hyperviscous and pseudo-parabolic regularization for the case of the time-dependent coefficients  $\mu = \mu(t)$ . We also mention that results concerning continuous dependence of solutions of the backward heat equation with different regularizing operators on the regularization parameters were proved in [3].

## 3.1 Hyperviscous Regularization

In this approach we take the regularization operator in the form of a sixth–order differential operator [1,3,14] i.e.,

$$\mathcal{B}_{\alpha}(\kappa) \triangleq \kappa^{6}, \tag{3.3}$$

although any higher–order operator in the form  $\kappa^{2m}$ ,  $m \ge 4$  could be used as well. The magnitude of this term is given by  $\mu = \alpha$ . As shown in Fig. 2a, when added to  $\mathcal{A}(\kappa)$ , this operator has the effect of attenuating Fourier modes  $\hat{p}_{\kappa}$  with  $\kappa > \sqrt{\frac{1+\sqrt{1-4\alpha}}{2\alpha}}$ , with the operator  $-\mathcal{A}_{\alpha}(\kappa) \triangleq -[\mathcal{A}(\kappa) + \mathcal{B}_{\alpha}(\kappa)]$  becoming stable for  $\alpha > 1/4$ . Moreover, we also observe that for  $\alpha > 1/3$  the peak in  $-\mathcal{A}_{\alpha}(\kappa)$  disappears and the spectrum of  $\mathcal{A}_{\alpha}$  becomes a monotonously decreasing function of  $\kappa$ . Thus, in a linear problem, given the spectral content of the terminal condition  $\varphi$ , one would be able to determine the minimum value of the regularization parameter  $\alpha$  required for stability and determine also the errors with respect to the unperturbed solution. Performance of this regularization strategy on our nonlinear problem will be assessed in Section 4. We add that for systems defined on a bounded domain it would be necessary to provide additional boundary conditions for regularization operator (3.3), and the choice of these boundary conditions is rather nonobvious.

#### 3.2 *Pseudo–Parabolic Regularization*

In this approach the regularization operator will involve four derivatives in space in addition to one derivative in time [1,3,19,20,21]

$$\mathcal{B}_{\beta}(\kappa) \triangleq \kappa^4 \frac{d}{dt},$$
(3.4)

so that the regularized operator becomes

$$\mathcal{A}_{\beta}(\kappa) \triangleq \frac{\kappa^2 - \kappa^4}{1 + \beta \kappa^4}.$$
 (3.5)

The magnitude of this regularization term is given by  $\mu = \beta$ . We remark that, in contrast to the hyperviscous technique, this approach to regularization also affects the form of the nonlinear term which becomes  $\hat{q}_{\kappa} = \frac{\left(p\frac{\partial p}{\partial \kappa}\right)_{\kappa}}{1+\beta\kappa^4}$ . Furthermore, the regularized operator  $\mathcal{A}_{\beta}(\kappa)$  is not given as a polynomial, but a rational function of  $\kappa$ . We note that restriction of  $\beta$  to positive values is necessary to avoid poles in expression (3.5) which could lead to undesirable behavior. To be more precise, for  $\beta < 0$ such poles would occur at the wavenumber  $\kappa_p \triangleq \sqrt[4]{-1/\beta}$  for which the denominator in (3.5) vanishes. As a result, operator  $\mathcal{A}_{\beta}(\kappa)$  would become unbounded for  $\kappa \to \kappa_p$  resulting in a "resonance" behavior which is clearly an undesirable effect. As is evident form Fig. 2b, the spectrum of the operator  $\mathcal{A}_{\beta}(\kappa)$  is now bounded for all  $\kappa$  by  $\beta^{-1}$ , but the operator remains unstable for all  $\beta$ . In this sense, regularized problem (3.2) with the regularization operator given in (3.4) still remains ill–posed, although, as shown by the computational results presented in Section 4, the degree of ill–posedness is weak and does not prevent an efficient numerical solution for moderate times. In principle, this ill–posedness could be mitigated by using higher–order spatial derivatives in (3.4) which would ensure that  $\mathcal{A}_{\beta}(\kappa) \rightarrow 0$ for  $\kappa \rightarrow \infty$ , but this was found unnecessary in the present investigation. We add that, since regularization operator (3.4) does not increase the order of the equation, for systems defined on bounded domains it is not necessary to provide additional boundary conditions in the pseudo–parabolic approach.

# 3.3 Adaptive Regularization

It appears plausible that an optimal value of the regularization parameter may change in time, hence a natural generalization of the approaches presented in Sections 3.1 and 3.2 is to allow the regularization parameters  $\alpha$  and  $\beta$  to be adapted in some dynamic fashion. As a criterion of this adaptation one may require that the solution of the regularized backward problem (3.2) have a prescribed fixed energy  $E_0$  given in terms of the  $L_2$  norm as as

$$||p(t)||_{L_2} \triangleq \int_0^L p(t,x)^2 dx = \sum_{\kappa \in \mathbb{K}} |\hat{p}_{\kappa}|^2 = E_0.$$
 (3.6)

The idea behind this admittedly simple criterion is to ensure that the regularization is not too "soft", resulting in an instability and blow–up, and at the same time not too aggressive, which could result in large errors. Condition (3.6) could be enforced at every discrete time step  $t_j$ ,  $j = N_T, ..., 1$ , where  $N_T$  is the total number of time steps, yielding

$$\|p(t_j; \mu(t_j))\|_{L_2} = E_0 \text{ for } t_j \in [0, T],$$
(3.7)

which can be solved for  $\mu(t_j)$  at every time  $t_j$  using a suitable root–finding technique. Alternatively, the rather rigid condition (3.7) can be relaxed and replaced with

$$||p(t;\mu(t))||_{L_2} \to E_0 \text{ as } t \to 0.$$
 (3.8)

Values of the regularization parameter  $\mu$  satisfying the weaker condition (3.8) can be determined using methods originating in the classical control theory [23], namely, a proportional (P) regulator

$$\mu(t_j) = \mu(t_{j+1}) + K_P\left(\|\hat{p}(t_{j+1};\mu(t_{j+1}))\|_{L_2} - E_0\right),$$
(3.9)

or a proportional-differential (PD) regulator

$$\mu(t_j) = \mu(t_{j+1}) + K_P \left( \| \hat{p}(t_{j+1}; \mu(t_{j+1})) \|_{L_2} - E_0 \right) + K_D \frac{d}{dt} \left( \| \hat{p}(t_{j+1}; \mu(t_{j+1})) \|_{L_2} - E_0 \right),$$
(3.10)

where  $K_P$  and  $K_D$  are adjustable parameters. Some results concerning adaptive hyperviscous and pseudo–parabolic regularization will also be presented in Section 4.

# 4 Computational Results

In this Section we assess the performance, both in terms of stability and accuracy, of the regularization methods introduced in Sections 3.1–3.3. We will do this by analyzing the divergence of the trajectory obtained by solving the regularized terminal value problem (3.2) from the "reference" trajectory corresponding to the original terminal value problem (3.1) in which no disturbances are present. This reference trajectory is in fact obtained by solving initial value problem (2.1) and using the state u(T) as the terminal condition for the backward problem (3.2), i.e.,  $\varphi = u(T)$ . Divergence of these two trajectories is characterized by the relative error

$$e(t) \triangleq \frac{\|p(t) - u(t)\|_{L_2}}{\|u(t)\|_{L_2}} \simeq \frac{\sqrt{\sum_{\kappa \in \mathbb{K}} |\hat{p}_{\kappa}(t) - \hat{u}_{\kappa}(t)|^2}}{\sqrt{\sum_{\kappa \in \mathbb{K}} |\hat{u}_{\kappa}(t)|^2}},$$
(4.1)

and we will be primarily interested in the studying the behavior of e(0). We also considered errors defined in terms of norms other than  $L_2$  (e.g.,  $H^1$  and  $H^{-1}$ ), but the results obtained were qualitatively similar and therefore will not be shown here. Both forward and backward problems (2.1) and (3.2) are discretized in space using a pseudo–spectral Fourier–Galerkin method with dealiasing [4]. We used 512 Fourier modes and found this sufficient to resolve fully all the investigated cases. Time discretization employed an implicit (Crank–Nicolson) scheme on all the linear (including regularization) terms in (2.1) and (3.2) combined with an explicit (RK3) scheme on the nonlinear terms. The time step used in the solution of both problems, regardless of the regularization technique used, was the same and equal to  $\Delta t = 2.9 \cdot 10^{-2}$ . We are primarily interested in the effect of nonlinearities represented by the parameter *L* in (1.1) and (1.2). In order to assess the performance of both regularization strategies in different regimes, for all values of *L* we study the problem on two different time intervals:

- (1) short time interval with  $T = 30 \cdot \Delta t$ ,
- (2) long time interval with  $T = 300 \cdot \Delta t$ .

For every value of *L* we ensure that the terminal condition  $\varphi$  lies on the "turbulent" attractor, so that the reference trajectory is guaranteed to exist (cf. discussion in Section 1) and the system evolution occurs in a statistically steady regime.

We begin our presentation of the results by showing in Figs. 3a,b and 4a,b the values of the relative error e(0) at the beginning of the interval [0,T] as a function of the regularization parameter ( $\alpha$  corresponding to the hyperviscous regularization in Figs. 3a,b, and  $\beta$  corresponding to the pseudo-parabolic regularization in Figs. 4a,b). We focus on the results defined at the beginning of the time window, because as shown in Fig. 5, the errors tend to be the largest there. Furthermore, for applications to the retrograde data assimilation [5,18] solution accuracy of the backward-in-time problem is the most important at t = 0. In order to facilitate



Fig. 3. The relative errors e(0) in the hyperviscous regularization as a function of the regularization parameter  $\alpha$  on (a) the short interval and (b) long interval with (•) L = 49, (**▲**) L = 154, (**■**) L = 267 and (**♦**) L = 462; figure (c) represents (solid line) the initial condition  $\phi$  of (1.1) and the states p(0) obtained by solving problem (3.2) with the hyperviscous regularization over (dotted line) the short interval and (dashed line) long interval for L = 154.

qualitative comparisons of the results in the different cases we used the same vertical scale in all four Figures. We note that the qualitative trends are the same for the two regularization methods on both the short and long interval. As the regularization parameters  $\alpha$  and  $\beta$  are reduced, the errors e(0) steeply increase which corresponds to an instability taking place due to insufficient regularization. For both regularization methods the critical value of the regularization parameter below which blow-up occurs is smaller for the short time interval, which indicates that the required "intensity" of regularization is an increasing function of the length of the integration interval. On the other hand, for increasing values of the regularization parameters the errors slowly grow indicating that due to excessive regularization the backward solutions deviate too far from the reference trajectory. In all four cases shown in Figs. 3a,b and 4a,b there is a well-defined value of the regularization parameter which yields a global minimum of the error e(0). These errors are noticeably smaller when the pseudo-parabolic regularization is used, and are also smaller on the short time intervals. In particular, when the pseudo-parabolic regularization is applied on the short interval, the relative error e(0) can as small as  $O(10^{-2})$ . These observations are confirmed in Figs. 3c and 4c where we compare the regularized solutions obtained at t = 0 using the "optimal" values of  $\alpha$  and  $\beta$  to the reference initial condition  $\phi$  (in order to magnify details only half of the domain [0,L] is shown in Figs. 3c and 4c). With regard to Fig. 4c, we reiterate that the solution obtained with the pseudo-parabolic regularization on the short time interval is barely distinguishable from  $\phi$ . Finally, we discuss the effect of the parameter L on the performance of the regularization strategies. We observe that in all of the four cases shown the errors corresponding to different L seem to collapse onto one curve (there is admittedly some scatter in the case of the pseudo-parabolic regularization). This rather surprising observation may imply a "universal" behavior of the two regularization techniques where L does not affect the performance.



Fig. 4. The relative errors e(0) in the pseudo-parabolic regularization as a function of the regularization parameter  $\beta$  on (a) the short interval and (b) long interval with (•) L = 49, (**(**) L = 154, (**(**) L = 267 and (**(**) L = 462; figure (c) represents (solid line) the initial condition  $\phi$  of (1.1) and the states p(0) obtained by solving problem (3.2) with pseudo-parabolic regularization over (dotted line) the short interval and (dashed line) long interval for L = 154.



Fig. 5. Comparison of the relative error e(t),  $t \in [0, T]$ , in the pseudo–parabolic regularization over the long interval using (solid line) a fixed value of  $\beta = 1.6$ , (dotted) "instantaneous" adaptation [cf. (3.7)], (dashed) adaptation using a P controller [cf. (3.9)], and (dash–dotted) adaptation using a PD controller [cf. (3.10)] for L = 154.

We conclude this Section with a discussion of the regularization results obtained with the adaptive technique introduced in Section 3.3. To fix attention, we focus on the pseudo–parabolic regularization applied on the long interval. We set  $E_0 = ||\varphi||_{L_2}$ and choose the constants  $K_P$  and  $K_D$  to ensure rapid convergence of  $||p(t)||_{L_2}$  to  $E_0$ as the time decreases. Numerous computational experiments did not produce an adaptive approach that would have been superior to the pseudo–parabolic regularization with a fixed  $\beta$  in the sense of yielding a smaller value of e(0). Sample results are presented in Fig. 5 where we see that, while for the intermediate times the adaptive approaches may perform marginally better, at the time t = 0 the approach with a fixed  $\beta$  is in fact superior.

## 5 Summary and Conclusions

In this paper we revisited two regularization techniques initially developed in the context of the backward–in–time heat equation, and applied them to a terminal value problem for a nonlinear system. Using the 1D backward–in–time Kuramoto–Sivashinsky equation as a model problem we showed that choosing optimal values of the regularization parameters involves a trade–off between stability and accuracy with integrations over shorter intervals requiring weaker regularization and yield-ing therefore more accurate results. The pseudo–parabolic regularization clearly performs much better than the hyperviscous regularization. It would furthermore be less ambiguous for problems defined on bounded domains, as it would not require additional boundary conditions to be specified (which would be the case for the hyperviscous regularization). We also found that, at least for problems evolving on the "turbulent" attractor, the parameter L has no systematic effect on the performance of the regularization techniques. This was rather unexpected, since L is

a measure of the nonlinear effects which in the Kuramoto–Sivashinsky system are of the advective type (thus, increasing *L* one reduces the relative significance of the dissipative terms which are the source of the backward–in–time ill–posedness).

Since the properties of the two regularization techniques are fully understood for linear problems, it would be tempting to compare our present results with regularization applied to problem (3.1) with the nonlinear term removed. Since such system does not possess a "turbulent" attractor, such a comparison would not be meaningful, because one would have to compare regularizations of transient and statistically stationary trajectories. In regard to applications in the retrograde data assimilation which have motivated this research, we conclude that the pseudo– parabolic regularization could be a feasible solution provided the integration intervals are sufficiently short.

## Acknowledgements

This work was carried out as the first author's M.Sc. research project. The financial support from McMaster University, in addition to funding from NSERC–Discovery (Canada), is gratefully acknowledged. The authors also wish to thank Thomas Bewley for many interesting discussions.

# References

 K. A. Ames, On the comparison of solutions of related properly and improperly posed cauchy problems for first order operator equations, SIAM Journal on Mathematical Analysis 13 (4) (1982) 594–606.

- [2] K. A. Ames, L. E. Payne, Asymptotic behavior for two regularizations of the cauchy problem for the backward heat equation, Mathematical Models and Methods in Applied Science 8 (1998) 187–202.
- [3] K. A. Ames, L. E. Payne, Continuous dependence on modeling for some well-posed perturbations of the backward heat equation, Journal of Inequalities and Applications 3 (1) (1999) 51–64.
- [4] C. Canuto, M. Y. Hussaini, A. Quarteroni, T. A. Zang, Spectral Methods: Fundamentals in Single Domiains, Springer, 2006.
- [5] J. Cessna, C. Colburn, T. Bewley, Multiscale retrograde estimation and forecasting of chaotic nonlinear systems, in: Proceedings of the 46th IEEE Conference on Decision and Control, 2007.
- [6] V. M. Eguíluz, P. Alstrøm, E. Hernández–García, O. Piro, Average patterns of spatiotemporal chaos: A boundary effect, Phys. Rev. E 59 (1999) 2822–2825.
- [7] H. Fujisaka, T. Yamada, Theoretical Study of a Chemical Turbulence, Progress of Theoretical Physics 57 (1977) 734–745.
- [8] M. D. Gunzburger, Perspectives in flow control and optimization, SIAM, 2003.
- [9] J. M. Hyman, B. Nicolaenko, The Kuramoto–Sivashinsky equation: a bridge between pdes and dynamical systems, Physica D 18 (1986) 113–126.
- [10] E. Kalnay, Atmospheric Modeling, Data Assimilation and Predictability, Cambridge University Press, 2003.
- [11] I. Kukavica, On the behavior of solutions of the Kuramoto-Sivashinsky equation for negative time, Journal of Mathematical Analysis and Applications 166 (1992) 601– 606.
- [12] I. Kukavica, M. Malcok, Backward behavior of solutions of the Kuramoto-Sivashinsky equation, Journal of Mathematical Analysis and Applications 307 (2005) 455–464.

- [13] Y. Kuramoto, Diffusion-Induced Chaos in Reaction Systems, Progress of Theoretical Physics Supplement 64 (1978) 346–367.
- [14] R. Lattés, J. L. Lions, The method of quasi-reversibility, Applications to partial differential equations, Elsevier, 1969.
- [15] W. Muniz, H. de Campos Velho, F. Ramos, A comparison of some inverse methods for estimating the initial condition of the heat equation, Journal of Computational and Applied Mathematics 103 (1999) 145–163.
- [16] W. Muniz, F. Ramos, H. de Campos Velho, Entropy– and Tikhonov–based regularization techniques applied to the backwards heat equation, Computers and Mathematics with Applications 40 (8-9) (2000) 1071–1084.
- [17] Y. Pomeau, A. Pumir, P. Pelce, Intrinsic Stochasticity with Many degrees of Freedom, Journal of Statistical Physics 37 (1-2) (1984) 39–49.
- [18] J.-P. Puel, A nonstandard approach to a data assimilation problem and tychonov regularization revisited, SIAM J. Control Optim. 48 (2009) 1089–1111.
- [19] R. E. Showalter, The final value problem for evolution equations, J. Math. Anal. Appl. 47 (1974) 563–572.
- [20] R. E. Showalter, Quasi–Reversibility of the first and second order parabolic evolution equations, in: A. Carasso, A. P. Stone (eds.), Improperly posed boundary value problems, Research Notes in Mathematics, Pitman, 1975.
- [21] R. E. Showalter, T. W. Ting, Pseudoparabolic partial differential equations, SIAM Journal on Mathematical Analysis 1 (1) (1970) 1–26.
- [22] G. Sivashinsky, Nonlinear analysis of hydrodynamic instability in laminar flames, Acta Astronautica 4 (1977) 1177–1206.
- [23] I. Vajk, State space control, chap. 2, CRC Press, 2005, pp. 393–404.

[24] R. W. Wittenberg, P. Holmes, Scale and space localization in the Kuramoto– Sivashinsky equation, Chaos 9 (1999) 452–465.