USING 1D-IRBFN METHOD FOR SOLVING A HIGH-ORDER NONLINEAR DIFFERENTIAL EQUATION ARISING IN MODELS OF ACTIVE-DISSIPATIVE SYSTEMS

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Abstract. We analyse a nonlinear partial differential equation modelling reaction-diffusion systems with nonlocal coupling and reaction fronts of gasless combustion. The equation is of active-dissipative type, nonlinear, with 6th-order spatial derivative. To numerically solve the equations we use the one-dimensional integrated radial basis function network (1D-IRBFN) method. The method has been previously developed and successfully applied to several problems such as structural analysis, viscous and viscoelastic flows and fluid-structure interaction. A commonly used approach is to differentiate a function of interest to obtain approximate derivatives. However, this leads to a reduction in convergence rate for derivatives and this reduction is an increasing function of derivative order. Accordingly, differentiation magnifies errors. To avoid this problem and recognising that integration is a smoothing process, the proposed 1D-IRBFN method uses the integral formulation, where spectral approximants are utilised to represent highest-order derivatives under consideration and then integrated analytically to yield approximate expressions for lower-order derivatives and the function itself. Our preliminary results demonstrate good performance of the 1D-IRBFN algorithm for the equation under consideration. Numerical solutions representing travelling waves are obtained, in agreement with the earlier studies.

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1 INTRODUCTION

The following model presents a single-equation simulation tool for certain type of active systems with dissipation,

$$\partial_t u = -A(\partial_x u)^2 \partial_x^2 u + B(\partial_x u)^4 + C\partial_x^6 u, \tag{1}$$

$A, B, C > 0$. In particular, Eq. (1) simulates combustion waves (fronts) having the shape of one or more steps [1] and developing instabilities in nonlocal reaction-diffusion systems [2]. In the context of combustion waves, u stands for the distance, measured along, say, axis z, passed by the combustion front through a hollow cylinder, as a function of the coordinate x and time t. The equation generates a rich variety of dynamical regimes, the most spectacular of which is the spinning wave illustrated by Fig. 1(a),(b). The graph (b) shows the wave solution of (1) simulating the experiment (a). On the graph the cylinder is rolled out into a plane and two periods are shown. The moving x locations of the steepest sections in figure (b) correspond to luminous spots spinning along the cylinder, due to extremely high temperatures.
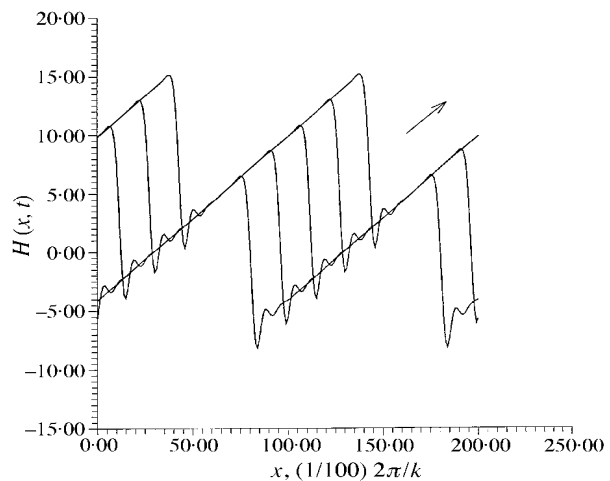
Figure 1: (a) A post-combustion trace on a hollow cylinder. (b) A running spinning wave solution of Eq. (1) (five successive shapes) evolved from a random initial condition [1].

Previously Eq. (1) has been solved numerically in 1D – with one independent spatial dimension x – using the spectral Galerkin method [1] and in 2D using a straightforward finite difference scheme. In this paper we aim to apply a different numerical method, which has proved to be fast and accurate in a number of problems, namely the 1D-IRBFN method. First we would like to test the method. Eq. (1) is unlikely to allow analytical solutions because of the nonlinearity, so we intend to obtain a single-step- travelling wave and compare it with the results shown in Fig. 1. In this figure we see a train of fronts, each comprising a sharp step followed by a long nearly flat shoulder. Although the shoulders appear inclined, their slopes

are much flatter than the abrupt steps. The speed of the front or steps, their height and width are controlled by the equation and not initial conditions. This is a consequence of the steps being formed as a result of the balance between the energy release in the system, represented by the term $-A(\partial_x u)^2 \partial_x^2 u$, and the dissipation, represented by the term $C \partial_x^6 u$. The term $B(\partial_x u)^4$ carries the function of the bridge between the above two. Our modelling in this paper is the first step in a new series of numerical exercises targeting various dynamical regimes generated by Eq. (1).

Note that by re-scaling t, x and u, Eq. (1) can always be transformed into a canonical form where all the coefficients, A, B, and C, become equal to 1.

2 THE NUMERICAL METHOD

The 1D-IRBF and IRBF-based methods have been successfully verified previously through several engineering problems such as turbulent flows [3], laminar viscous flows [4, 5, 6], structural analysis [7], and fluid-structure interaction [8].

Radial basis function networks (RBFNs) have been known as powerful high-order approximation tools for scattered data [9]. A function $f(\mathbf{x})$, to be approximated, can be represented by an RBFN as

$$f(\mathbf{x}) \approx u(\mathbf{x}) = \sum_{i=1}^{N} w_i G_i(\mathbf{x}), \qquad (2)$$

where $\mathbf{x}$ is the input vector, N the number of RBFs, $\{w_i\}_{i=1}^{N}$ the set of network weights to be found, and $\{G_i(\mathbf{x})\}_{i=1}^{N}$ the set of RBFs. According to Micchelli's theorem, there is a large class of RBFs, e.g. the multiquadric, inverse multiquadric and Gaussian functions, whose design/interpolation matrices obtained from (2) are always invertible. It has been proved that RBFNs are capable of representing any continuous function to a prescribed degree of accuracy. Furthermore, according to the Cover theorem, the higher the number of RBFs used, the more accurate the approximation will be, indicating the property of "mesh convergence" of RBFNs. Among RBFs, the multiquadric functions ($G_i(\mathbf{x}) = \sqrt{(\mathbf{x} - \mathbf{c}_i)^\top (\mathbf{x} - \mathbf{c}_i) + a_i^2}$, $\mathbf{c}_i$ - the centre and a_i - the width) are ranked as the most accurate and possess an exponential convergence with the spatial discretisation refinement.

The application of RBFNs for solving partial differential equations has received wide attention over the last decades (e.g. [10] and references therein). The usual approach [11, 12] is to differentiate (2) as often as required to obtain approximate derivatives of $f(\mathbf{x})$. If the error in $f(\mathbf{x})$ is $O(h^s)$, where h is the mesh size and $s > 0$, the error in the nth derivative of $f(\mathbf{x})$ is $O(h^{s-n})$. In other words, there is a reduction in convergence rate for derivatives and this reduction is an increasing function of derivative order. Thus, differentiation will magnify any error that might exist in the approximation of $f(\mathbf{x})$.

To avoid this problem, recognising that integration is a smoothing process, the integral formulation was proposed [13, 14], where spectral approximants (e.g. RBFNs) are utilised to represent highest-order derivatives under consideration and then integrated analytically to yield approximate expressions for lower-order derivatives and the function itself, to construct the ap-

proximations for the field variables in a problem. This approach was called integrated radial basis function networks or IRBFN. Although RBF methods can be easily implemented in a truly meshless manner based on scattered data points, it proves very efficient and effective to discretise a domain using Cartesian grids. Thus, the purpose of using integration (a smoothing operator) to construct the approximants is to avoid the reduction in convergence rate caused by differentiation, and also to improve the numerical stability of a discrete solution.

The integration process naturally gives rise to arbitrary constants that serve as additional expansion coefficients, and therefore facilitate the employment of some extra equations in the process of converting the RBF weights into the function values as illustrated above. This distinguishing feature of the integral formulation provides effective ways to overcome well-known difficulties associated with conventional differential approaches: (i) the implementation of multiple boundary conditions [15]; (ii) the description of non-rectangular boundaries on a Cartesian grid [16]; (iii) the imposition of high-order continuity of the approximate solution across subdomain interfaces [17]; and (iv) the incorporation of nodal derivative values into the approximations via compact IRBFN stencils (C-IRBFN) [18, 19]. The ability of the IRBFN methods to capture very sharp gradients, which is highly desirable for Eq. (1), has been demonstrated with the effective simulation of shockwave-like behaviours as in the dynamic strain localisation in a quasi-brittle material subjected to a sudden step loading [20].

3   RESULTS OF THE NUMERICAL EXPERIMENT: SETTLING OF THE TRAVELLING FRONT

Figures 2–3 show a sequence of snapshots displaying the solution of Eq. (1) evolving from the initial condition chosen in the step-like (front-like) form

$$u(x, 0) = 8 \exp[-(x - 5)^2] \text{ for } x \geq 5,$$

$$u(x, 0) \equiv 8 \text{ for } x < 5.$$

The idea is to help the solution curve acquire the step-like shape hinted by Fig. 1, although we realise that ultimate settled configuration of the solution will not depend of the initial condition.

In our numerical experiments we chose not to transform the equation to the canonical form, in order to be able to adjust the coefficient values as necessary, for example to increase or reduce the energy release in the system in hope to achieve a self-sustained balance between the release and dissipation. The parameter values were: $A = 5$, $B = 1$, $C = 1$, the number of nodes 401, the length of the x-interval 10, time step $2 \cdot 10^{-6}$. The x-interval was constantly shifted to the right to follow the main kink, which, according to the initial shape, was to move to the right. When looking at Fig. 1(b), if one stretches the x-axis enough, the long shoulders would become nearly horizontal. In fact each shoulder could stretch to infinity on both sides of an isolated single step. Aiming at such a solution, we adopt the boundary conditions

$$\partial_x u = 0, \quad \partial_x^2 u = 0, \quad \partial_x^3 u = 0$$

on the left and right ends of the (moving) x-interval.
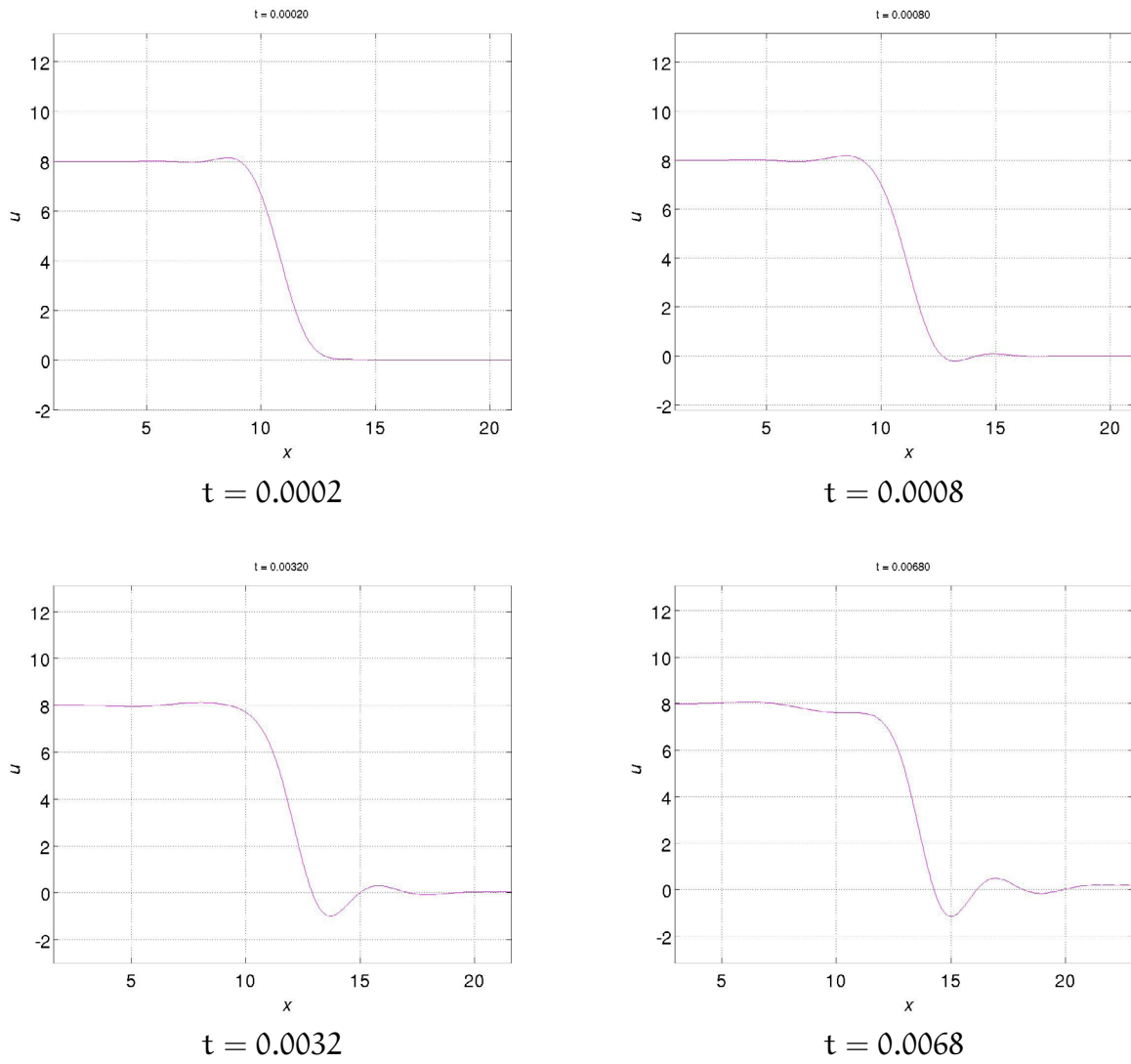
Figure 2: Evolving solution of Eq. (1) via the 1D-IRBFN method.
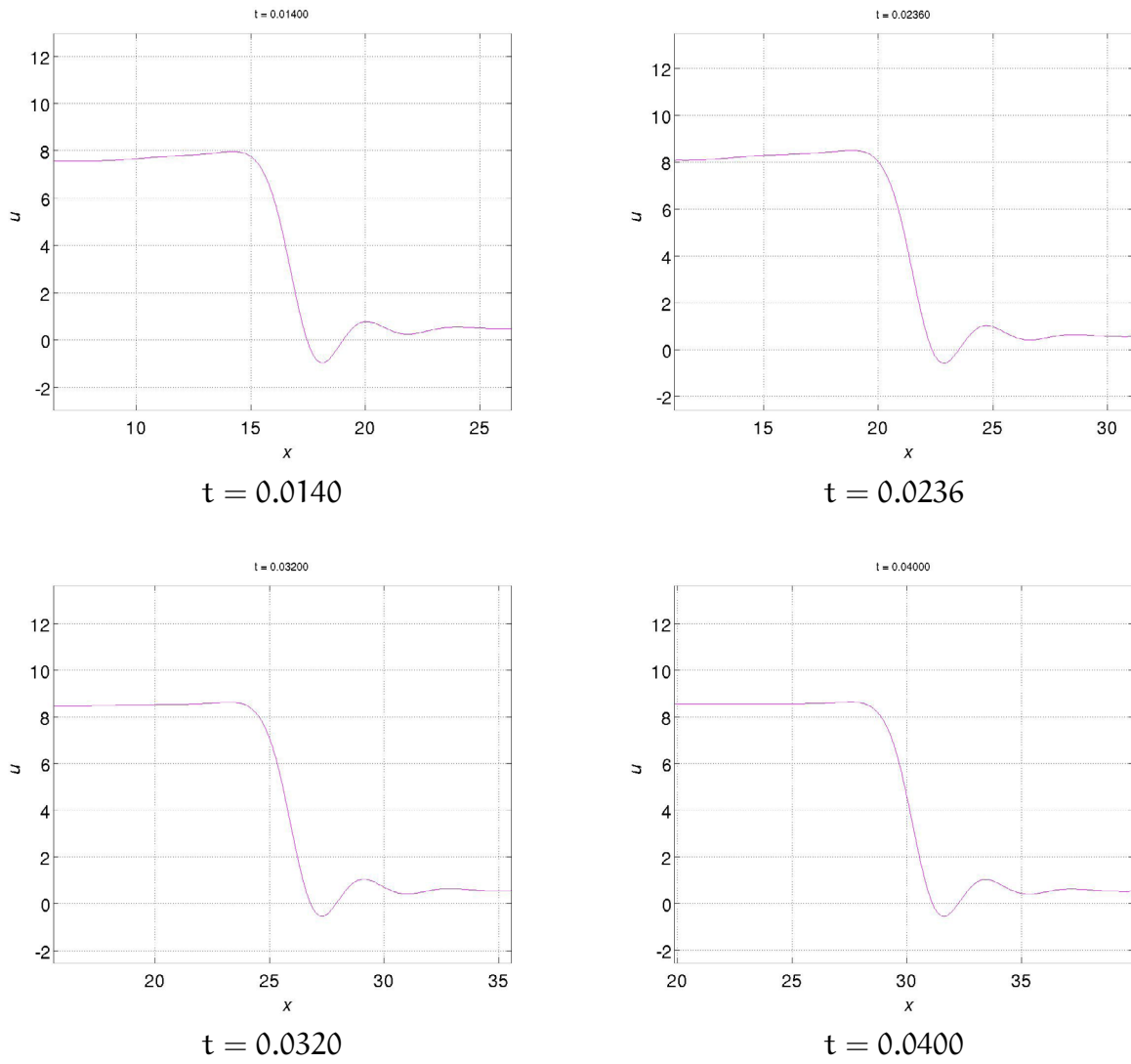
Figure 3: Evolving solution of Eq. (1) via the 1D-IRBFN method.

The experiment showed that after some period of transitional evolution lasted from $t_0 = 0$ to about $t = 0.03$, the curve practically ceased changing in shape. Continuing the experiments further gave the same frozen shape of the solution moving with constant speed to the right. Looking at the solution displayed in Fig. 1(b) we see the same characteristic tale of ripples in front of the main kink. They were expected to form, caused by the high order of the dissipation acting in the system. Immediately in front of the main kink sits a shorter one, followed, as we look from left to right, by barely distinguishable smaller ripples. The height of the main kink relative to its neighbour is about 4:1 or a bit higher, for the both figures. The fact that the solution settles into a steady moving shape of correct proportions correlates with the earlier result.

4   CONCLUSIONS

We applied the 1D-IRBF numerical method to solve Eq. (1) simulating spinning combustion fronts and oscillations in certain class of reaction-diffusion systems. To our satisfaction, the method produced a similar shape of the settled travelling front as the earlier study [1]. We plan to use the 1D-IRBF approach to study more complicated regimes such as co-directed motion of several fronts, collision of counter-directed fronts etc.

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