Numerical Solutions for PDEs Modeling Binary Alloy Solidification Dynamics

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Abstract. This paper studies the Shivashinsky equation with periodic boundary conditions using the finite difference and the wavelet-Galerkin discretization. It is proved that the schemes are uniquely solvable.

1. Introduction

We consider the nonlinear evolutionary problem governed by the famous Sivashinsky equation [13] modeling a planar solid-liquid interface for a binary alloy. We propose some numerical approximations based on the order reduction method to solve the following periodic-value problem.

\[
\begin{align*}
\frac{\partial u}{\partial t} + \alpha \frac{\partial^4 u}{\partial x^4} + \frac{\partial^2 f(u)}{\partial x^2} &= 0, \quad x \in [0,1], \quad t \in [0,T], \\
u(x,0) &= u_0(x), \quad x \in [0,1].
\end{align*}
\]

(1)

where \(u\) is a real-valued function 1-periodic in the space, \(u_0\) is a given 1-periodic function, \(f(u) = \frac{1}{2} u^2 - 2u\). Such problem and analogous versions have been the object of many studies especially those dealing with numerical approaches. This is due to the relationship of such problems with natural, physical, chemical phenomena... For an interesting review on such subjects and applications we refer to [3], [8]-[11], [14]-[17], where numerical interests on wind ripple, Sivashinsky equation, shock wave, viscous pumps, hydropulser mechanisms, electrospinning and dendrite growth

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were provided. In the present paper, we use a reduction order procedure. We then set \( v = f(u) - \frac{\partial^2 u}{\partial x^2} \).

So, problem (1) will be transformed to the following splitting equivalent system.

\[
\begin{align*}
\frac{\partial u}{\partial t} + \alpha u &= \frac{\partial^2 v}{\partial x^2}, \quad x \in [0, L], \quad t \in [0, T], \\
v &= f(u) - \frac{\partial^2 u}{\partial x^2}, \quad x \in [0, L], \quad t \in [0, T],
\end{align*}
\]

(2)

with the boundary and initial conditions

\[
u(0, t) = u(1, t) , \quad v(0, t) = v(1, t) \quad \text{and} \quad u(x, 0) = u_0(x), \quad x \in \Omega.
\]

We develop a semi-implicit finite difference scheme and wavelet-Galerkin approximation.

2. Finite difference method

Let \( M \) and \( N \) be integers. We fix a space step \( h = 1/M \) and a time one \( \Delta t = T/N \). We seek a solution in the space

\[
W = \{ v = (v_i) \subset \mathbb{R} ; \quad v_{i+1} = v_i , \quad i \in \mathbb{Z} \}.
\]

For \( u \in W \) and \( v_1, v_2, \ldots, v^n, \ldots \in W \) we use the discrete operators

\[
\Delta_h u_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} \quad \text{and} \quad \frac{\partial}{\partial t} v^n = \frac{v^n - v^{n-1}}{\Delta t}.
\]

We shall also use the discrete inner product

\[
(u, v) = h \sum_{i=1}^{M} u_i v_i , \quad u, v \in W
\]

and the associated discrete norm. We finally denote \( u^n_i \) the net function \( u(ih, n\Delta t) \). The idea consists in using an implicit scheme for the linear term and an explicit one for the nonlinear. We then seek \( (u^n, v^n) \in W^2 \) such that

\[
\begin{align*}
\Delta_h u_i^n + \alpha u_i^n &= \Delta_h v_i^n , \quad 0 \leq i \leq M, \quad 0 \leq n \leq N, \\
v_i^n &= f(u_i^{n-1}) - \Delta_h u_i^n , \quad 0 \leq i \leq M, \quad 1 \leq n \leq N, \\
u_i^0 &= u_0(ih) , \quad 1 \leq i \leq M.
\end{align*}
\]

(3)

This yields a matrix form

\[
\begin{align*}
(1 + \alpha \Delta t) U^n - U^{n-1} &= -\Delta A V^n , \quad 1 \leq n \leq N, \\
V^n &= F(U^{n-1}) + A U^n , \quad 1 \leq n \leq N, \\
U^0 &= \text{given}.
\end{align*}
\]

(4)

where \( U^n, V^n \) and \( F(U^n) \) are the vectors whom components are respectively

\[
U_i^n = u_i^n , \quad V_i^n = v_i^n \quad \text{and} \quad F(U)_i = f(u_i^n).
\]

2
$A$ is the $M \times M$ matrix whom coefficients are given by

$$A(i,i) = -2 \text{ and } A(i-1,i) = A(i,i+1) = A(1,M) = A(M,1) = 1.$$ 

**Theorem 2.1**

1. The system (3) has a unique solution.
2. Suppose that the solution $u$ of (2) is sufficiently smooth. For $k$ sufficiently small, the solution of the difference scheme (3) converges to the solution $u$ by means of the discrete $L^2$-norm at the rate $o(h^2 + k)$.

The proof of the first point is based on the theory of circulant matrices. We transform the system (4) into a circulant invertible-matrix equivalent system. The second point is based on Taylor error truncations and some technical computations.

3. **Wavelet-Galerkin approach**

The method is based on Daubechies periodized compactly supported wavelets. Let $\phi$ be a Daubechies scaling function supported on the interval $[0,L-1]$. The periodized scaling function at the scale $J$ and the position $k$ is defined by

$$\phi_{J,k}^{\text{per}}(x) = 2^{J/2} \sum_{s \in \mathbb{Z}} \phi(2^J(x - s) - k).$$

Define the approximation space at level $J$ by

$$V_J = \left\{ w \in L^2(0,1); \ w = \sum_{k \in \mathbb{Z}} w_{J,k} \phi_{J,k}^{\text{per}}, \ w_{J,k} = w_{J,k+2^J} \right\}.$$

The wavelet-Galerkin approximation of the solution $(u,v)$ at the scale $J$ is

$$u_J(x,t) = \sum_{k \in \mathbb{Z}} u_{J,k}(t) \phi_{J,k}^{\text{per}}(x) \text{ and } v_J(x,t) = \sum_{k \in \mathbb{Z}} v_{J,k}(t) \phi_{J,k}^{\text{per}}(x).$$

By substituting the expansions of $u_J$ and $v_J$ into (2) and taking the inner product of both sides with $\phi_{J,s}^{\text{per}}, s \in \mathbb{Z}$ we obtain

$$\begin{align*}
(1 + \alpha \Delta t)u_{J,s}^n - u_{J,s}^{n-1} &= \Delta t 2^{2J} \sum_{k \in \mathbb{Z}} v_{J,k}^n \Gamma_{s-k} \\
v_{J,s}^n &= F(u_{J,s}^{n-1}) - 2^{2J} \sum_{k \in \mathbb{Z}} u_{J,k}^n \Gamma_{s-k}
\end{align*}$$

(7)

where

$$\Gamma_{s-k} = \int_0^1 (\phi_{J,s}^{\text{per}})(x) \phi_{J,k}^{\text{per}}(x) dx \text{ and } F(u_{J,s}^{n-1})(x) = \int_0^1 f(u_{J,s}^{n-1}(x)) \phi_{J,s}^{\text{per}}(x) dx.$$

We then obtain a circulant matrix system of the form

$$\begin{align*}
(1 + \alpha \Delta t)U_J^n - U_J^{n-1} &= \Delta t A_J V_J^n \\
V_J^n &= F(U_J^{n-1}) - A_J U_J^n.
\end{align*}$$

(8)

$A_J$ is the symmetric circulant matrix of order $p = 2^J$ its first column is given by

$$A_J(:,1) = 2^{J/2} (\Gamma_0, \Gamma_1, \ldots, \Gamma_{L-2}, \Gamma_{L-1}, 0, 0, \ldots, \Gamma_{2-L}, \Gamma_{3-L}, \ldots, \Gamma_{-J})^T.$$
Theorem 3.1
1. The system (7) is uniquely solvable.
2. Suppose that the solution \( u \) of (2) is sufficiently smooth. The solution of the discrete scheme (7) converges to the solution \( u \) by means of the discrete norm at the rate \( 2^{-\mu/2} \).

4. Numerical Implementations
The first method based on finite difference scheme is not complicated, and its implementation does not yield difficult problems. However, the second method has yielded an important problem related to the computation of derivatives on wavelets and so of the connection coefficients

\[
\Gamma_{i-j} = \int_0^1 (\varphi_{ij}^{\text{per}})^n(x) \varphi_{ij}^{\text{per}}(x) \, dx
\]

Such integrals play an important role in the wavelet-Galerkin method for solving differential equations since in general there are no explicit expressions for representing scaling functions and their derivatives. For this reason, these integrals have been the object of several studies such as [2]. In such a reference, a standard study has been provided to compute the \( n \)-th order derivation integrals instead second-order. Whereas, the author in [2] has provided the values only for the one-order derivation in the case of Daubechies compactly supported scaling function. Such a choice is justified by the fact that the considered problems are on bounded domains. The problem of providing a general derivation adopted algorithm remains open. In [1], the author developed a more sophisticated algorithm to compute general integrals of the form

\[
\Gamma^n_{i}(x) = \int_0^x \varphi(t-i)\varphi^{(n)}(t) \, dt
\]

for \( x \) and \( n \) integers. The idea was by resolving an eigenvalue problem. The author provided some reduction in the number of the coefficients of the obtained matrix system and he proved that a reduced number of the integrals is sufficient to compute all of them. The numerical results exposed in [2] have been re-tested.

In our work, we also used Daubechies compactly supported wavelets. We recall that we seek a 1-periodic solution of problem (1). This is why we consider the periodized scaling functions. To compute the values of the derivation integrals \( \Gamma_{i-j} \) we applied the techniques of [1]. Denote \( n=i-j \). One has immediately

\[
\Gamma_{i-j} = \sum_{l \in \mathbb{Z}} r_{i-j+n} \text{ where } r_i = \int_{-\infty}^{\infty} \varphi(x-s)\varphi''(x) \, dx.
\]

Analogous but modified techniques are applied to evaluate the nonlinear operator \( F(u) \). Here we apply also the techniques of [1] combined with [7] for computing the three-term connection coefficient of wavelets

\[
\Omega_{j,k}^{m,n} = \int_{-\infty}^{\infty} \varphi_{j}^{\text{per}}(y)(\varphi_{j}^{\text{per}})^{(m)}(y-j)(\varphi_{j}^{\text{per}})^{(n)}(y-k) \, dy
\]

The nonlinear term is obtained by

\[
F(u_{j,k}) = -2u_{m,j} + \frac{1}{2} \sum_{k \in \mathbb{Z}, k \neq j} u_{j,k} b_{j,k} b_{j-k,j-k-j}
\]

where

\[
b_{m,n} = 2^{j/2} \sum_{l \in \mathbb{Z}} \sum_{l' \in \mathbb{Z}} \Omega_{m-n-2,l, l'}^{0,0,0}.
\]
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