

ACCURATE SPECTRAL SOLUTIONS TO A PHASE-FIELD TRANSITION SYSTEM

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Abstract The paper is mainly concerned with numerical approximation of solutions to the phase-field transition system (Caginalp's model), subject to the non-homogeneous Dirichlet boundary conditions. Numerical approximation of solutions to the nonlinear phase-field (Allen-Cahn) equation, supplied with the non-homogeneous Dirichlet boundary conditions as well as with homogeneous Cauchy-Neumann boundary conditions is also of interest. To achieve these goals, a Chebyshev collocation method, coupled with a Runge-Kutta scheme, has been used. The role of the nonlinearity and the influence of the boundary conditions on numerical approximations in Allen-Cahn equation were analyzed too. To cope with the stiffness of Caginalp's model, a multistep solver has been additionally used; all this, in order to march in time along with the same spatial discretization. Some numerical experiments are reported in order to illustrate the effectiveness of our numerical approach.

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1. INTRODUCTION

A great deal of qualitative and quantitative research has been done on the reaction-diffusion problems (see [16], [17] and references therein), in particular on the Allen-Cahn equation (see [1], [10], [11], [15]) and the phase-field transition system (see [4], [5], [6], [13]). For numerical investigations on the phase-field system and nonlinear Allen-Cahn equation, we refer to the works [2], [8], [12], [13], [14] and [15].

Up to our knowledge, the classical Allen-Cahn equation supplied with mixed boundary conditions has not been considered numerically. Thus our first aim is to fill this gap. Also we have to observe that a Lyapunov energy functional for this case is no longer available. We also generalize this model using high order polynomials as nonlinear terms. These polynomials conserve the dynamic of the classical Allen-Cahn model, i.e., $u = 0$ is an unstable state and $u = \pm 1$ are stable states. The periodic case has been recently addressed in [10].

In the second part we extend our analysis to a more involved model, namely the so called Caginalp model. This model adds to the previous nonlinearity a genuine

stiffness. In order to resolve this stiffness we make use of a multistep method of the numerical differentiation formula type. Our experience with spectral collocation gathered in the recent booklet [7] encouraged us to use this discretization method based on Chebyshev polynomials.

2. THE ALLEN-CAHN INITIAL-MIXED BOUNDARY VALUE PROBLEM

Let's consider the nonlinear initial-boundary value parabolic problem in $Q := [-1, 1] \times (0, T]$ with $T > 0$

$$\begin{cases} \tau \xi u_t = \xi u_{xx} + F(u) + g(x, t) & \text{in } Q, \\ -\xi u_x(-1, t) + c_0 u(-1, t) = \xi u_x(1, t) + c_0 u(1, t) = 0 & t \in (0, T], \\ u(x, 0) = u_0(x) & x \in (-1, 1), \end{cases} \quad (1)$$

where τ, ξ and c_0 are positive physical parameters. The problem is the 1D variant of the general formulation provided in [15]. Existence, uniqueness and regularity results are also available in this paper. Corresponding to simple Dirichlet problem, a recent paper is that of Miranville [11].

For the nonlinear term F , we have chosen the polynomial form (Allen-Cahn)

$$F(u) := \frac{1}{2\xi} (u - u^3), \quad (2)$$

and the *source term* g was considered as null in the first instance. The case of the greatest interest is that when the *measure of interface thickness* ξ is small, i.e. $0 < \xi \ll 1$.

A physical (correct) range of variation for *relaxation time* τ and for the *measure of interface thickness* ξ is suggested by the inequality (7) from Section 3.

2.1. CHC METHOD COUPLED WITH RUNGE-KUTTA

Chebyshev collocation (CHC for short) coupled with Runge-Kutta in order to solve problem (1) means to solve the system of ordinary differential equations

$$\begin{cases} \tau U_t = \tilde{D}^{(2)} U + \frac{U - U^3}{2\xi^2} & t \in (0, T], \\ U(X, 0) = u_0(X), \end{cases} \quad (3)$$

where:

- X is the set of the interior nodes of the usual Chebyshev-Gauss-Lobatto system x_0, x_1, \dots, x_N attached to the interval $[-1, 1]$;

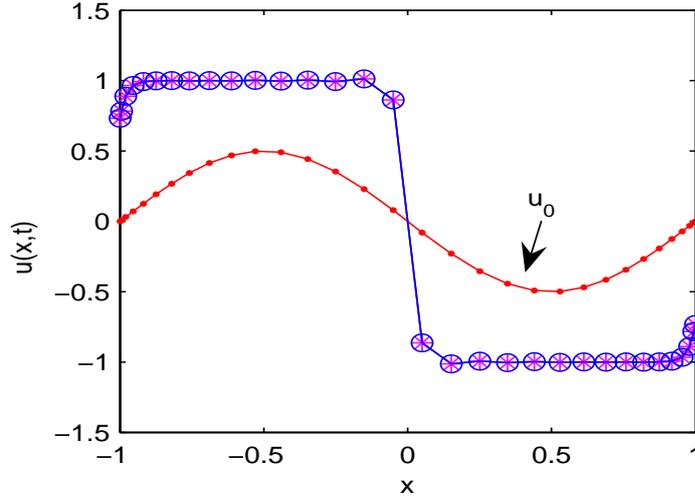


Fig. 1.: Solution to problem (1) when $N = 42$ and $T = 3/\pi$.

- $U(X, t)$ is the vector containing the approximations of solution u in the nodes X at the moment t , i.e., $u(x_1, t), \dots, u(x_{N-1}, t)$;
- $\widetilde{D}^{(2)}$ is the second order Chebyshev differentiation matrix with the mixed boundary conditions enforced (see [18]);
- in the r. h. s. of (3) as well as throughout this paper we will use the MATLAB conventions;

For $\tau := 1/10$, $\xi := 1/15$, $c_0 := 1$ and the initial data $u_0(x) := -\sin(\pi x)/2$ the solution to problem (1) is displayed in Figure 1. The mesh for of the solution obtained with the same values of the parameters but with initial data $u_0(x) := -\sin(2\pi x)/2$ is displayed in Figure 2.

The mixed boundary condition bent the graph of the solution close to both ends $x = \pm 1$. This is the visible effect of this type of boundary conditions.

2.2. THE STEADY STATE ALLEN-CAHN PROBLEM

The steady state mixed boundary value problem attached to Allen-Cahn equation reads

$$\begin{cases} \varepsilon u_{xx} + F_{SS}(u) + g(x) = 0, & x \in (-1, 1), & 0 < \varepsilon \ll 1, \\ -\varepsilon u_x(-1) + u(-1) = \varepsilon u_x(1) + u(1) = 0, \end{cases} \quad (4)$$

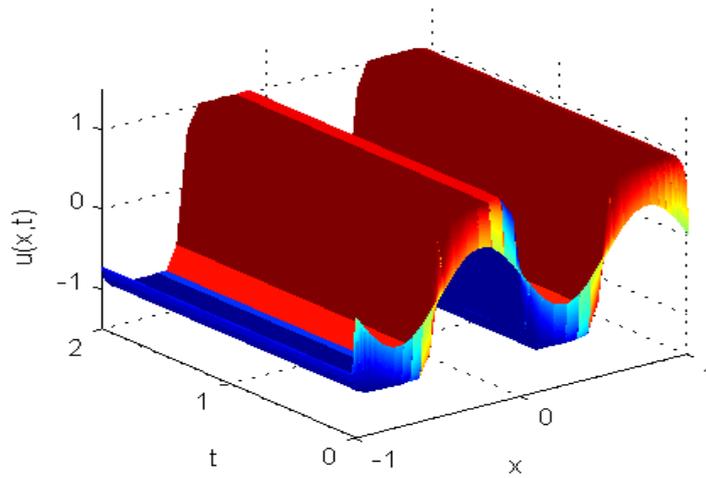


Fig. 2.: The mesh form of the solution to problem (1) when $N = 42$ and $T = 2$.

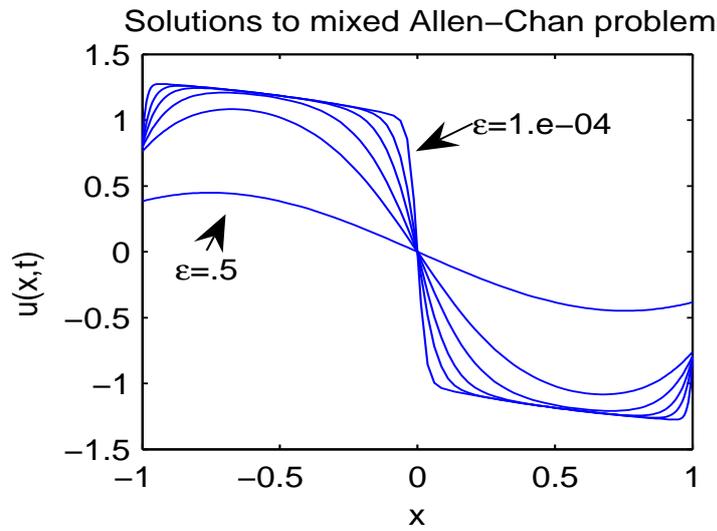


Fig. 3.: Solutions to steady state mixed boundary value problem attached to Allen-Cahn equation when $N = 128$.

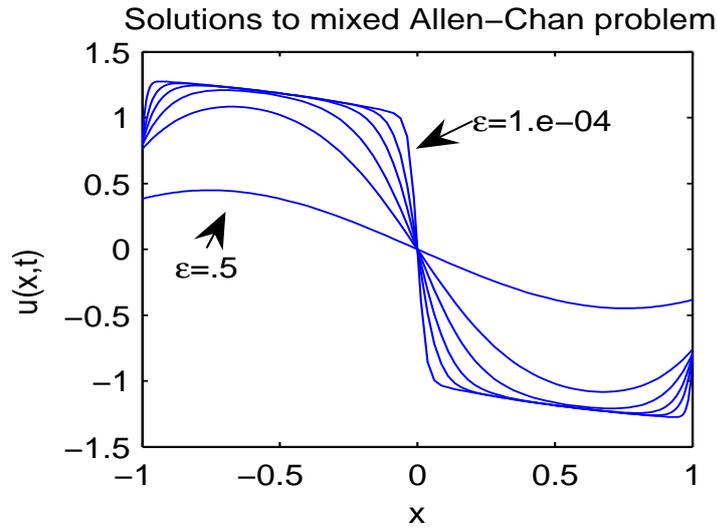


Fig. 4.: Solutions to steady state Dirichlet boundary value problem attached to Allen-Cahn equation.

where $F_{SS}(u) := u - u^3$. Some solutions of this problem for various ε and $g(x) := \sin(x)$ are depicted in Figure 3.

Using the MATLAB code `fsolve` we get convergent solutions for $64 \leq N \leq 512$ and various initial guesses. The steady state Dirichlet boundary value problem attached to Allen-Cahn equation differs from the above problem by the boundary condition, namely

$$u(-1) = u(1) = 0.$$

Some solutions of this problem for various ε and the same source term $g(x)$ and N are depicted in Figure 4. The numerical experiments carried out indicate a stable ChC procedure.

2.3. THE STEADY STATE ϕ^5 PROBLEM

Let's consider now the case $F_{SS}(u) := u - u^5$. The solution to mixed problem is depicted in Figure 5 and the solution to Dirichlet problem is displayed in Figure 6.

The difference between the last two cases consists in the fact that in the latter situation `fsolve` does not work for N larger than 32.

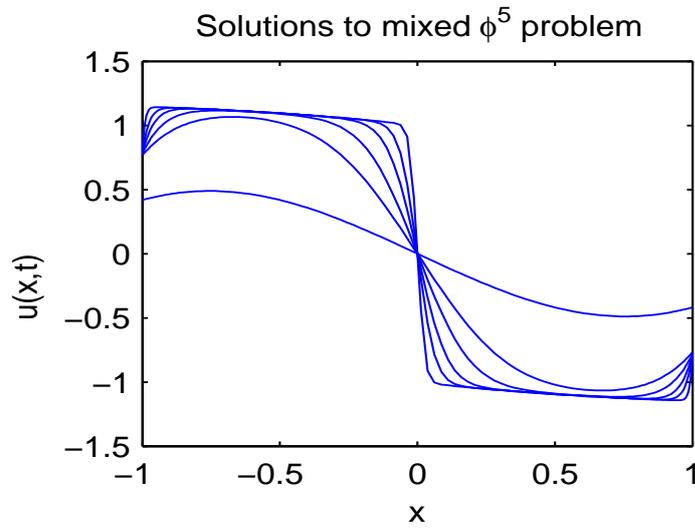


Fig. 5.: Some solutions to mixed ϕ^5 problem when $N = 128$ and $\xi = .5, .1, .03, .009, .003, .0005$.

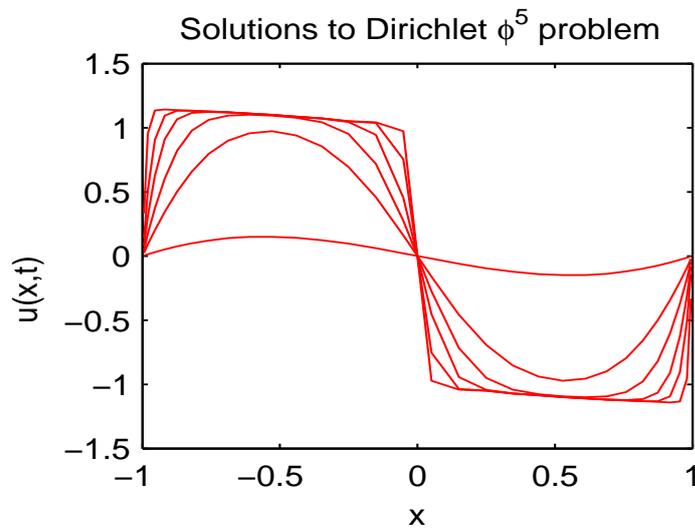


Fig. 6.: Some solutions to Dirichlet ϕ^5 problem when $N = 128$ and $\xi = .5, .1, .03, .009, .003, .0005$.

2.4. THE STEADY STATE ϕ^{2P+1} PROBLEM, $P = 3$

Let's consider a little bit modified problem to observe better the balance between *stiffness* and *nonlinearity*. The new problem reads

$$\begin{cases} u_t = \varepsilon u_{xx} + u - u^{2p+1}, & p \in \mathbb{N}, \quad 0 < \varepsilon \ll 1 & \text{in } Q, \\ u(-1, t) = -1, \quad u(1, t) = 1 & t \in (0, T], \\ u(x, 0) = u_0(x) & x \in (-1, 1). \end{cases} \quad (5)$$

In [9] this problem is solved in order to detect the *meta-stability phenomenon*. The authors use an *exponential integrator* as an alternative to implicit methods for the numerical solution of stiff PDEs. The method combine the exact solution of the linear part with the numerical resolution of the remaining, nonlinear part (see also [3]).

The solution to the problem (5) has been obtained by Chebyshev collocation applied to the linear term along with a time marching ETDRK4 scheme. It is fairly clear that the meta-stability persist in case of this nonlinear case, i.e. after a period of transition of order $t \approx 260$ the initial data transforms just into a solution with one interface between the attracting states $u = -1$ and $u = 1$.

It is fairly important to observe that this transition period increases along with the exponent p of nonlinearity. For instance, when $p = 1$, this transition period appears at $t = 40$.

3. THE CAGINALP'S MODEL

The physics of the solidification process (see [4], [8], [13]), leads to the following system of genuinely nonlinear parabolic differential equations

$$\Phi_t = A \Delta \Phi + F(\Phi), \quad (6)$$

where

$$\Phi := \begin{pmatrix} u \\ \varphi \end{pmatrix}, \quad A := \begin{pmatrix} K & -\frac{\ell \xi^2}{2\tau} \\ 0 & \frac{\xi^2}{\tau} \end{pmatrix},$$

and the source term is

$$F(\Phi) := \left[\frac{1}{2} (\varphi - \varphi^3) + 2u \right] \frac{1}{\tau} \begin{pmatrix} -\frac{\ell}{2} \\ 1 \end{pmatrix}.$$

The unknown φ is the so called *phase field function* and u is the difference between the temperature T and its melting value T_M i.e., $u(x, t) := T(x, t) - T_M(x, t)$. The

physical parameters ℓ , ξ , and τ stand respectively for *latent heat* per unit mass, *length scale* and *relaxation time*. K is the *thermal diffusivity* (see also [8], [13]).

In [4] the author has carried out a rigorous analysis concerning the existence and regularity of solutions of (6). Invariant regions of the solution space have also been obtained. He observes that the existence has been shown for fixed values of ξ and τ satisfying the *stability inequality*

$$0 < \frac{\xi^2}{\tau} < K. \quad (7)$$

He also remarks that one of the questions of interest is the behavior of these equations in the limit of *small* ξ and τ . Boundary as well as initial conditions have to be attached to (6). Actually, we have solved the initial-Dirichlet boundary value problem

$$\left\{ \begin{array}{ll} \Phi_t = A \Delta \Phi + F(\Phi) & x \in (-1, 1), \quad t \in (0, T), \\ \Phi(-1, t) = -1, \quad \Phi(1, t) = 1 & t \in (0, T), \\ \Phi(x, 0) = 0.53x + 0.47 \sin(-35\pi x/2) & x \in [-1, 1]. \end{array} \right. \quad (8)$$

In some of our numerical experiments we have used, as in Section 2.1 $\xi = 1/15$, $\tau = 1/10$ and then $K = 1$ and $\ell = 1$. However, in order to observe the behavior of the solutions of (6) for $\xi^2/\tau \rightarrow 0$ we also have considered this problem when $\xi^2/\tau = 10^{-3}$ ($\xi^2 = 10^{-2}$, $\tau = 10$). An analogous semi-discretized problem with that attached to Allen-Cahn equation, i.e., (3), but double as dimension, is used to solve (6).

The interval of time integration has been $T = 10$. In this case the problem is a fairly stiff one and consequently the Runge-Kutta integrator failed. The results presented in Fig. 8 and Fig. 9 have been carried out using the MATLAB code `ode15s` which is a multi-step solver based on a numerical differentiation formula.

However, this scheme for time marching along with ChC provided accurate numerical results. The main remark refers to the fact that in this case the transition to meta-stability is not so smooth as it has proved to be in Allen-Cahn case (compare Fig. 7 and Fig. 8).

The evolution of temperature variable is fairly predictable. After a short transition period, the initial sinusoidal perturbation becomes a linear variation between the *cold* or *solid* state and the *hot* or *liquid* one. In fact the temperature variable appears linearly in the system (6).

4. CONCLUDING REMARKS

The Chebyshev collocation along with Runge-Kutta scheme or a numerical differentiation scheme for the stiff Caginalp's model provided accurate solutions to the problems considered in this study. In both situations the algorithm is stable, i.e., provides identical results for values of the cut off parameter N in the range 2^5 and 2^8 .

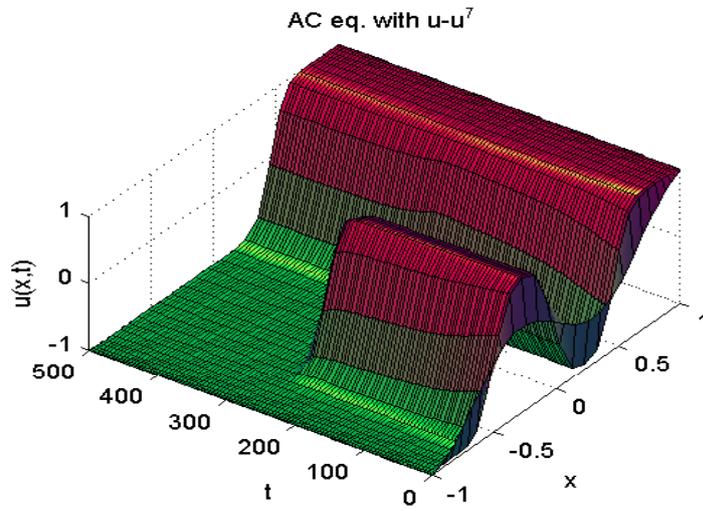


Fig. 7.: The solution to the problem (5) when $p = 3$, $\varepsilon = 0.01$ and $N = 32$.

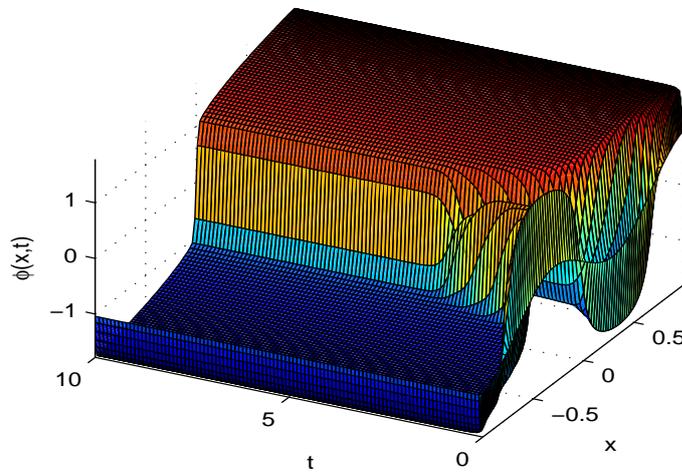


Fig. 8.: Phase-field function solution to problem (8) when $N = 128$.

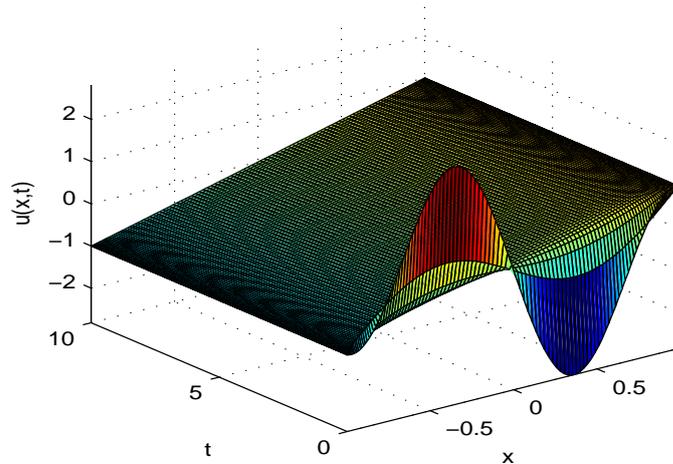


Fig. 9.: Temperature solution to problem (8) when $N = 128$.

The metastability phenomenon has been accurately captured in both Allen-Cahn and Caginalp's models. Neither the higher nonlinearities nor the mixed boundary conditions do not have modified significantly the behavior of solutions in the former model.

References

- [1] S. Allen, J.W. Cahn, *A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening*, Acta Metall., **27**(1979), 1084-1095.
- [2] V. Arnăutu, C. Moroşanu, *Numerical approximation for the phase-field transition system*, Intern. J. Com. Math., **62**(1996), 209-221.
- [3] H. Berland, B. Skaflestad, M.W. Will, *EXPINT- A MATLAB Package for Exponential Integrators*, ACM Trans. on Math. Software, **33**, Article 4, 2007.
- [4] G. Caginalp, *An Analysis of a Phase Field Model of a Free Boundary*, Arch. Rational Mech. Anal. **94**(1986), 205-245.
- [5] O. Cârjă, A. Miranville, C. Moroşanu, *On the existence, uniqueness and regularity of solutions to the phase-field system with a general regular potential and a general class of nonlinear and non-homogeneous boundary conditions*, Nonlinear Analysis - TMA, **113** (2015), 190-208.
- [6] C.M. Elliott, S. Zheng, *Global existence and stability of solutions to the phase field equations*, in Internat. Ser. Numer. Math., Birkhauser, Basel, **95**(1990), 46-58.
- [7] C.I. Gheorghiu, *Spectral Methods for Non-Standard Eigenvalue Problems. Fluid and Structural Mechanics and Beyond*, Springer Briefs in Mathematics, 2014.
- [8] Gh. Iorga, C. Moroşanu, I. Tofan, *Numerical simulation of the thickness accretions in the secondary cooling zone of a continuous casting machine*, Metalurgia International, **XIV**(2009), 72-75.

- [9] A-K. Kassam, L.N. Trefethen, *Fourth-Order Time Stepping for Stiff PDEs*, SIAM J. Sci. Comp., **26**(2005), 1214-1233.
- [10] H.G. Lee, J.-Y Lee, *A semi-analytical Fourier spectral method for the Allen-Chan equation*, DOI: 10.1016/j.camwa.2014.05.015
- [11] A. Miranville, *Existence of Solutions for a One-Dimensional Allen-Cahn Equation*, JAAC, **3**(2013), 265-277.
- [12] C. Moroşanu, *Approximation and numerical results for phase field system by a fractional step scheme*, Revue d'Analyse Numérique et de Théorie de l'Approximation, **25**, 1-2(1996), 137-151.
- [13] C. Moroşanu, *Analysis and optimal control of phase-field transition system: Fractional steps methods*, Bentham Science Publishers, <http://dx.doi.org/10.2174/97816080535061120101>, 2012.
- [14] C. Moroşanu, Ana-Maria Moşneagu. *On the numerical approximation of the phase-field system with non-homogeneous Cauchy-Neumann boundary conditions. Case 1D*, ROMAI J., **9**(2013) 91-110.
- [15] C. Morosanu, A. Croitoru, *Analysis of an iterative scheme of fractional steps type associated to the phase-field equation endowed with a general nonlinearity and Cauchy-Neumann conditions*, J. Math. Anal. Appl.(2015), <http://dx.doi.org/10.1016/j.jmaa.2015.01.033>.
- [16] C. V. Pao, *Nonlinear parabolic and elliptic equations*, Plenum Press, New York, 1992.
- [17] R. Temam, *Infinite Dimensional Dynamical Systems in Mechanics and Physics*, Springer, New York, 1997.
- [18] J.A.C. Weideman, S.C. Reddy, *A MATLAB Differentiation Matrix Suite*, ACM Trans. on Math. Software, **26**(2000), 465-519.