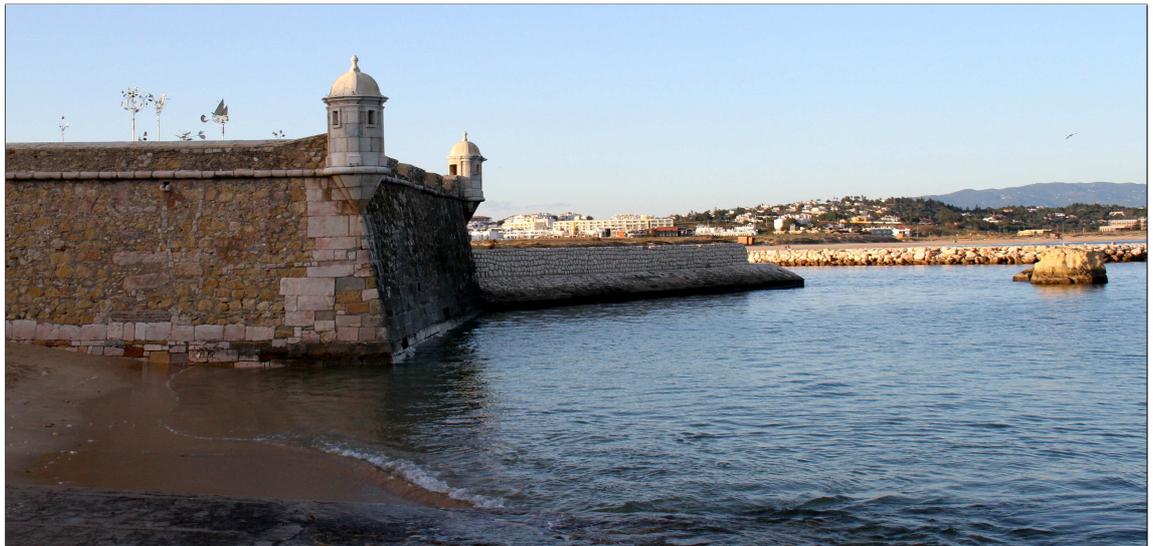


Fifth International Workshop on Analysis and Numerical  
Approximation of Singular Problems (IWANASP 2015)  
22-24 October, 2015 Lagos, Portugal

# Book of Abstracts





## BOOK OF ABSTRACTS

FIFTH INTERNATIONAL WORKSHOP ON ANALYSIS AND NUMERICAL  
APPROXIMATION OF SINGULAR PROBLEMS (IWANASP 2015)

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**1. FIRST PART: ABSTRACTS OF THE INVITED TALKS**

INVITED TALKS

## THE CHOICE OF BASIS FOR PROJECTION METHODS IN WEAKLY SINGULAR INTEGRAL EQUATIONS

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When considering a weakly singular Fredholm integral equation of the 2nd kind

$$T\varphi - z\varphi = f, \quad (1)$$

where  $z$  is in the resolvent set of  $T$ ,  $f \in X$ , and  $T : X \rightarrow X$ , is a compact linear integral operator on the space of Lebesgue integrable complex valued functions  $X$ , defined by

$$(T\varphi)(\tau) = \int_0^{\tau^*} g(|\tau - \tau'|)\varphi(\tau') d\tau', \quad (2)$$

we can use classical projection methods where Eq. (1) is replaced by

$$T_n\varphi_n - z\varphi_n = f, \quad (3)$$

$T_n$  being a Galerkin, Sloan (iterated Galerkin), Kantorovitch or Kulkarni approximation of  $T$  ( see [4]).

In the examples to be shown, kernel  $g$  can be either the  $-\log(s/2)$ ,  $s \in ]0, 2]$  kernel (see [3]) or the radiative transfer in stellar atmospheres kernel, as described in [1].

For the numerical solution of (3), using projection methods, the evaluation of a discretization matrix  $A_n$ , which represents the integral operator  $T_n$  restricted to a finite dimensional space  $X_n$ , is required.

The precision of the approximate solution depends, not only on the projection method used, but also on dimension of the discretization subspace, on the basis of this subspace, and on the precision of the evaluation of this discretization matrix.

The choice of the basis must take in account the properties of the space where the problem is set, and the discontinuities of the kernel and of the source term  $f$ .

For instance, for the second problem mentioned, [1] shows that  $X$  should be the Banach space  $L^1$  and the basis of  $X_n$  as simple as possible, but based on a grid that can include the discontinuities. In [2] and [3] some relations between the basis and the error on the solutions are shown for some projection methods. Here we will discuss other cases.

This is a joint work with Rosário Fernandes, from the University of Minho, Maria João Rodrigues, from the University of Porto, and Mario Ahues, from the University of Saint Etienne.

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## MATHEMATICAL MODELLING OF AUTOIMMUNITY

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The talk presents a model of  $\beta$ -cell transitions for diabetes. The normal  $\beta$  cells may die through apoptosis (a naturally occurring programmed death) or necrosis (where the cells die in an uncontrolled way resulting in a build-up of dead tissue and cell debris) which can lead to premature death in patients.

The model is based on a system of delay-differential equations and the aim of the project is to study the interactions and to understand how one may control cell death resulting from necrosis through the values of parameters of the system.

## CONSTRUCTION OF IMPLICIT-EXPLICIT DIMSIMS OF HIGH ORDER

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For many systems of differential equations modeling problems in science and engineering, there are often natural splittings of the right hand side into two parts, one of which is non-stiff or mildly stiff, and the other part is stiff. Such systems can be efficiently treated by a class of implicit-explicit (IMEX) diagonally implicit multistage integration methods (DIMSIMs), where the stiff part is integrated by implicit formula, and the non-stiff part is integrated by an explicit formula. We analyze stability of these methods when the implicit and explicit parts interact with each other. We look for methods with large absolute stability region, assuming that the implicit part of the method is  $A(\alpha)$ -,  $A$ -, or  $L$ -stable. Finally we furnish examples of IMEX DIMSIMs of order  $p = 5$  and  $p = 6$  with good stability properties. (This is a joint work with Hans Mittelmann).

## **NONLOCAL DIFFUSION, A MITTAG-LEFFLER FUNCTION AND A TWO-DIMENSIONAL VOLTERRA INTEGRAL EQUATION**

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In this paper we consider a particular class of two-dimensional singular Volterra integral equations. Firstly we show that these kind of equations can indeed arise in practice by considering a diffusion problem with an output flux which is nonlocal in time. This problem is shown to admit an analytic solution in the form of an integral. More crucially this problem can be re-characterized as an integral equation of this particular class. This example then provides motivation for a more general study: an analytic solution is obtained for the case when the kernel and the forcing function are both unity. This analytic solution, in the form of a series solution, is a variant of the Mittag-Leffler function. As a consequence it is an entire function. A Gronwall lemma is obtained. This then permits a general existence and uniqueness theorem to be proved.

## **THE MATHEMATICS OF AGEING: FROM THE HEART TO THE EYE**

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The transport of chemical molecules in body tissues depends on their properties but also on the physiological properties of the target tissues. A compromised elasticity, a larger stiffness, and an increased porosity are common characteristics of ageing tissues. The aim of this talk is to show how these properties influence the pharmacokinetics of drugs.

Mathematical models, composed by systems of partial differential equations and integro-differential equations, that represent the coupling between drug delivery devices and body tissues, are presented. Theoretical results concerning the qualitative behavior of the systems will be presented. Numerical simulations show the predictive value of the models.

This is a joint work with J. Ferreira and P. Silva from CMUC and J. Naghipoor from the University of Weimar, Germany.

## CHARACTERIZATION OF FRACTIONALLY DIFFERENTIABLE FUNCTIONS

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We study the existence of the Riemann-Liouville, Caputo a.o. fractional derivatives of a given function. Let us formulate a result about Caputo differentiability. Denote by  $\mathcal{H}_0^\alpha[0, T]$ ,  $0 < \alpha < 1$ , the closed subspace of the standard Hölder space  $\mathcal{H}^\alpha[0, T]$ :

$$v \in \mathcal{H}_0^\alpha[0, T] \text{ iff } \sup_{0 \leq s < t \leq T, t-s \leq \varepsilon} |v(t) - v(s)| (t-s)^{-\alpha} \rightarrow 0 \text{ as } \varepsilon \rightarrow 0$$

**THEOREM 1.** For  $v \in C^m[0, T]$ ,  $m \in \mathbb{N}_0 = \{0, 1, 2, \dots\}$ ,  $m < \alpha < m + 1$ , the following conditions (i), (ii), (iii) are equivalent:

(i) the fractional derivative  $D_{\text{Cap}}^\alpha v \in C[0, T]$  exists;

(ii) a finite limit  $\lim_{t \rightarrow 0} t^{m-\alpha} (v^{(m)}(t) - v^{(m)}(0)) =: \gamma_m$  exists, and the Riemann improper integrals  $\int_{\theta t}^t (t-s)^{m-\alpha-1} (v^{(m)}(t) - v^{(m)}(s)) ds$ ,  $0 < t < T$ , equiconverge:

$$\sup_{0 < t \leq T} \left| \int_{\theta t}^t (t-s)^{m-\alpha-1} (v^{(m)}(t) - v^{(m)}(s)) ds \right| \rightarrow 0 \text{ as } \theta \uparrow 1;$$

(iii)  $v^{(m)}$  has the structure  $v^{(m)} - v^{(m)}(0) = \gamma_m t^{\alpha-m} + v_m$  where  $\gamma_m$  is a constant,  $v_m \in \mathcal{H}_0^{\alpha-m}[0, T]$ , and  $\int_0^t (t-s)^{m-\alpha-1} (v^{(m)}(t) - v^{(m)}(s)) ds =: w_m(t)$  converges for every  $t \in (0, T]$  defining a function  $w_m \in C(0, T]$  with a finite limit  $\lim_{t \rightarrow 0} w_m(t) =: w_m(0)$ .

For  $v \in C^m[0, T]$  with  $D_{\text{Cap}}^\alpha v \in C[0, T]$ , it holds  $(D_{\text{Cap}}^\alpha v)(0) = \Gamma(\alpha + 1 - m)\gamma_m$ ,

$$(D_{\text{Cap}}^\alpha v)(t) = \frac{1}{\Gamma(m+1-\alpha)} \left( t^{m-\alpha} (v^{(m)}(t) - v^{(m)}(0)) \right. \\ \left. + (\alpha - m) \int_0^t (t-s)^{m-\alpha-1} (v^{(m)}(t) - v^{(m)}(s)) ds \right), \quad 0 < t \leq T.$$

The results are used in treating the Abel equation (with a coefficient function) and in numerical methods for it.

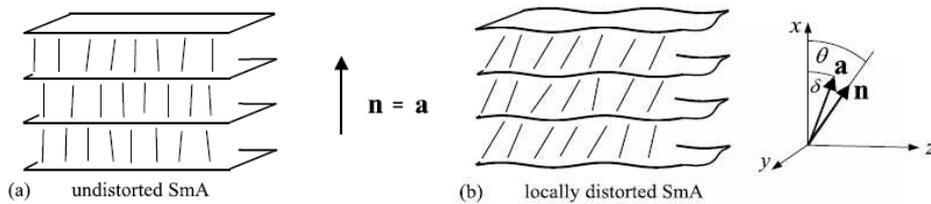
# THE SINGULAR-PERTURBATION ASYMPTOTICS AND NUMERICS OF FLOW IN SMECTIC A LIQUID CRYSTALS

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**Figure 1.** (a) A schematic diagram of locally arranged planar layers of SmA liquid crystal. In an undistorted configuration in the bulk, away from any boundary influences, the layers prefer to be equidistant and the local layer normal  $\mathbf{a}$  coincides with the director  $\mathbf{n}$ . (b) The layer and director alignments may be perturbed from their preferred undistorted orientations in which case  $\mathbf{a}$  and  $\mathbf{n}$  need no longer coincide. The orientation angles  $\theta$  and  $\delta$ , for  $\mathbf{n}$  and  $\mathbf{a}$ , respectively, are measured relative to the direction of the undistorted layer normal.

Smectic A (SmA) liquid crystals are fluid, layered, materials which obey Darcy's law for flow normal to the layers and Navier Stokes equations in the other two directions [1, 2]; a schematic of the structure in undistorted and distorted configurations is given in Fig. 1. Distortions can occur either due to the influence of boundaries or because of flow, and are quantified through two orientation angles,  $\theta$  and  $\delta$ , that are measured relative to the direction of the undistorted layer normal.

This contribution considers the analysis of a mathematical model for flow driven by a pressure gradient applied to SmA liquid crystals between two plates in a direction normal to the layers. Asymptotic analysis quantifies the width of boundary layers in  $\theta$  and  $\delta$  at the plates, but also indicates the presence of a transition layer through which  $\theta$  and  $\delta$  change from their undistorted bulk values. Comparison is made with the corresponding analysis when there is no pressure gradient, and the analysis is then reconciled for both cases with the results of numerical computations.

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## COLLOCATION – AN EFFICIENT TOOL FOR SOLVING SINGULAR ODES AND DAES

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During recent years, a lot of scientific work concentrated on the analysis and numerical treatment of boundary value problems (BVP) in ordinary differential equations (ODEs) which can exhibit singularities. Such problems have often the following form:

$$y'(t) = \frac{1}{t}M(t)y(t) + f(t, y(t)), \quad t \in (0, 1], \quad b(y(0), y(1)) = 0,$$

where  $f$  is assumed to be appropriately smooth. Here, we will focus on the slightly more difficult situation, where the functions  $f$  is unsmooth,  $f(t, y(t)) = g(t, y(t))/t$ ,  $g$  smooth. We first deal with the analytical properties of the problem, existence and uniqueness of smooth solutions, especially with the most general boundary conditions which guarantee its well-posedness.

The search for efficient numerical methods to solve the above BVP is strongly motivated by numerous applications from physics, chemistry, mechanics, ecology, or economy. In particular, problems posed on semi-infinite intervals,  $[0, \infty)$  are frequently transformed to a finite domain taking above form with the leading term  $M(t)y(t)/t^\alpha$ ,  $\alpha > 1$ . Also, research activities in related fields, like differential algebraic equations (DAEs) or singular Sturm-Liouville eigenvalue problems benefit from techniques developed for singular BVPs.

The method of choice for the numerical solution of the singular ODEs is polynomial collocation which is robust with respect to the singularity and retains its advantageous convergence properties known for regular ODEs. For collocation at equidistant points or Gaussian points this convergence results mean that the scheme with  $m$  inner collocation points constitutes a high order basic solver whose global error is  $O(h^m)$  uniformly in  $t$  [5]. Due to the robustness of collocation, this method was used in one of the best established standard FORTRAN codes for (regular) BVPs, COLSYS, as well as in Matlab codes `bvp4c`, the standard module for (regular) ODEs with an option for singular problems, `BVP SOLVER`, `sbvp` [1], and `bvpsuite` [6]. The scope of `bvpsuite` includes fully implicit form of the ODE system with multi-point boundary conditions, arbitrary mixed order of the differential equations including zero, module for dealing with infinite intervals, module for eigenvalue problems, free parameters, and a path-following strategy for parameter-dependent problems with turning points. We will illustrate how `bvpsuite` can be used to solve BVPs from applications [2].

Finally, we turn to DAEs. Especially, higher index DAEs constitute a really challenging class of problems due to the differentiation involved in the solution process which is a critical operation to carry out numerically. A possible technique to master the problem is to pre-handle the DAE system in such a way that the transformed problem is of index 1 and less difficult to solve. Since this approach is technically involved, it is worth to try to avoid it and provide a method which can be applied directly to the original DAE system of high index. We will first discuss the easier index-1 case for which analytical results are already available and then illustrate the performance of the least squares collocation for higher index DAEs [3, 4].

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## A FAST FOURIER–GALERKIN METHOD SOLVING A BOUNDARY INTEGRAL EQUATION FOR THE BIHARMONIC EQUATION

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We develop a fast Fourier–Galerkin method for solving a boundary integral equation which is a reformulation of the Dirichlet problem of the biharmonic equation. The proposed method is based on a splitting of the resulting boundary integral operator. That is, we write the operator as a sum of two integral operators, one having the Fourier basis functions as eigenfunctions and the other whose representation matrix in the Fourier basis can be compressed to a sparse matrix having only  $\mathcal{O}(n \log n)$  number of nonzero entries, where  $n$  is the order of the Fourier basis functions used in the method. We then project the solution of the boundary integral equation onto the space spanned by the Fourier basis functions. This leads to a system of linear equations. A fast solver for the system is based on a compression of its coefficient matrix. We show that the method has the optimal convergence order  $\mathcal{O}(n^{-q})$ , where  $q$  denotes the degree of regularity of the exact solution of the boundary integral equation and requires computing only  $\mathcal{O}(n \log n)$  number of entries of the coefficient matrix. Numerical examples are presented to confirm the theoretical results for the approximation accuracy and computational complexity of the proposed method.

## 2. SECOND PART: ABSTRACTS OF THE CONTRIBUTED TALKS

### CONTRIBUTED TALKS

## NUMERICAL METHODS FOR A CLASS OF NONLINEAR SINGULAR SECOND KIND VOLTERRA INTEGRAL EQUATIONS

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We consider the numerical solutions to some nonlinear singular Volterra integral equations which arise in applications such as: boundary value problems of heat transfer between solids and gases, theory of superfluidity and the temperature distribution on the surface of a projectile moving through a laminar layer (Lighthill's equation). These equations contain a weakly singular kernel of the form  $s^\beta(t-s)^{-\alpha}$ , with  $\alpha \in (0, 1)$  and  $\beta > 0$ , where in general their solutions are not regular [4]. The typical nonsmooth properties of the exact solution to these equations cause a drop in the global convergence orders of numerical methods with uniform meshes like collocation or product integration methods. It is known that spectral methods are suitable for equations with smooth solutions (see [2]). A new transformation is introduced in order to transform the original equation into the one with smooth solution. The errors in the spectral approximation to the new equation decay exponentially in  $L^\infty$ -norm and weighted  $L^2$ -norm. Some numerical examples are presented to illustrate the theoretical results. Other numerical methods like the Galerkin spectral method are also proposed.

This is joint work with T. Diogo and M. Rebelo.

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## **METHOD OF MULTIPLE SHOOTING FOR ODE BOUNDARY VALUE PROBLEMS AND APPLICATION FOR FINDING GEOMETRIC SHORTEST PATHS**

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Method of multiple shooting is well-known for solving ODE boundary value problems. It includes the factors: discretization of the domain, refinement of shooting points to ensure the continuity and differentiability of the solution of these problems. In this talk we present geometric aspects of these factors and apply for finding shortest paths between two points inside a simple polygon or on the surface of a convex polytope in a three dimensional space. Numerical results are given. This is a joint work with N. N. Hai and T. V. Hoai.

## SINGULAR POLYNOMIAL SYSTEMS

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According to [2, 3], a system of multivariate polynomial equations is called singular if it has a zero manifold of positive dimension which disappears under almost all perturbations of the system. A typical case is a system of  $n$  polynomials in  $n$  variables subject to a small perturbation,

$$p_i(z) + \epsilon q_i(z) = 0, \quad z = (z_1, \dots, z_n), \quad i = 1 \dots n, \quad (1)$$

with the property that the unperturbed system (with  $\epsilon = 0$ ) admits a zero manifold, while for the perturbed system (with  $\epsilon \neq 0$ ) only a finite number of isolated zeros  $z(\epsilon)$  survive. This means that for  $\epsilon \approx 0$  the  $z(\epsilon)$  are necessarily ill-conditioned and may be difficult to retrieve. Now the question is whether it is possible to localize the zeros  $z(\epsilon)$  by considering the unperturbed system and identifying points  $z(0)$  on the zero manifold which approximate nearby values  $z(\epsilon)$ , filtering out ‘nonapproximating zeros’ on the manifold.

We present an ideal-theoretic approach to this type of problems which has been developed in [1]. The following elimination algorithm is proposed:

- Introduce  $\eta$  ( $= 1/\epsilon$ ) as a new variable and augment (1) by the equation  $p_0 := \epsilon \eta = 1$ .
- Eliminate the variable  $\eta$  from the ideal generated by  $p_0, p_1, \dots, p_n$ .
- In the resulting ideal, set  $\epsilon = 0$ , simplify, and solve the polynomial system defined by the basis elements of the outcome.

We present the ideas from [1] and give several examples illustrating the successful performance of the proposed algorithm. Nontrivial examples are handled using Gröbner basis computations in a computer algebra system for the ideal-theoretic manipulations.

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# APPLICATION OF THE $\varepsilon$ -APPROXIMATE FIXED-POINT METHOD TO SOLVING BOUNDARY VALUE PROBLEMS FOR SECOND ORDER SINGULARLY DISTURBED DELAY DIFFERENTIAL EQUATIONS

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The presentation will be devoted to numerical solution of boundary value problems for second order singularly perturbed delay differential equations of the form

$$\varepsilon y''(x) = f(x, y(x), y'(x), y(\alpha(x))), \quad a \leq x \leq b, \quad (1)$$

$$y(x) = \phi(x) \quad \text{for } x \leq a, \quad y(b) = \psi. \quad (2)$$

where the functions  $f$ ,  $\phi$  and  $\alpha$ ,

$$f : D \rightarrow R, \quad D = \{(t, z_1, z_2, z_3) : a \leq t \leq b, -\infty \leq z_i \leq +\infty\},$$

$$\phi : [\gamma, a] \rightarrow R, \quad \alpha : [a, b] \rightarrow (-\infty, b], \quad \gamma = \min_{a \leq x \leq b} \alpha(x)$$

are continuous and  $0 < \varepsilon \ll 1$ . Problem (1) – (2) is reduced to a fixed-point problem of the form

$$y = Ay, \quad (3)$$

which is approximated by a fixed-point problem in a finite dimensional space

$$y_h = A_h y_h. \quad (4)$$

Problem (4) is solved by the  $\varepsilon$ -approximate fixed-point method described in [1].

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## SOLUTIONS STRUCTURE OF SINGULAR NONLINEAR SECOND ORDER ODE

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We investigate the singular nonlinear second order ordinary differential equation

$$(p(t)u'(t))' + q(t)f(u(t)) = 0, \quad (1)$$

on unbounded domain  $[0, \infty)$  subject to initial conditions

$$u(0) = u_0 \in [L_0, L], \quad u'(0) = 0, \quad (2)$$

where the interval  $[L_0, L]$  is related to the continuous function  $f$  with three zeros  $f(L_0) = f(0) = f(L) = 0$ ,  $L_0 < 0 < L$  and the sign conditions  $xf(x) > 0$  for  $x \in (L_0, 0) \cup (0, L)$ . Further,  $p, q \in C[0, \infty)$  are positive on  $(0, \infty)$  and  $p(0) = 0$ . The integral  $\int_0^1 \frac{ds}{p(s)}$  may be divergent which yields the time singularity at  $t = 0$ .

Our aim is to describe the set of all solutions of problem (1), (2). We define three different types of solutions according to their asymptotic behaviour. By means of results concerning their existence and other properties, we proceed to the existence of a monotonously increasing solution satisfying the boundary conditions

$$u'(0) = 0, \quad \lim_{t \rightarrow \infty} u(t) = L. \quad (3)$$

This solution, called the bubble-type solution, plays an important role in applications. For  $p \equiv q = t^{N-1}$ , where  $N$  is the space dimension, equation (1) is called the density profile equation and together with the boundary conditions (3) describes the formation of microscopic bubbles in a nonhomogeneous fluid. A numerical investigation of the problem can be found for example in [2].

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# A NYSTRÖM METHOD FOR INTEGRAL EQUATIONS WITH FIXED SINGULARITIES OF MELLIN TYPE IN WEIGHTED $L^P$ SPACES

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We propose a numerical method for approximating the solutions of integral equations of the following type

$$f(y) \pm \int_0^1 \frac{1}{x} \bar{k}\left(\frac{y}{x}\right) f(x) dx + \int_0^1 h(x, y) f(x) dx = g(y), \quad y \in (0, 1], \quad (1)$$

where  $\bar{k} : [0, +\infty) \rightarrow [0, +\infty)$  is a given function satisfying suitable assumptions,  $h(x, y)$  and  $g$  are given smooth functions and  $f$  is the unknown.

Such type of equations are of interest because appears in several problems of mathematics, physics and engineering. For example they occur when boundary integral methods are used on domains with corners (see e.g. [1, 2, 5] and the references therein). Due to the presence of a Mellin type kernel  $\frac{1}{x} \bar{k}\left(\frac{y}{x}\right)$  having a fixed-point singularity at  $x = y = 0$ , the standard stability proofs for numerical methods do not apply and, then, a modification of the classical methods in a neighbourhood of the endpoint  $y = 0$  is needed.

Following [7, 6, 4, 3] we propose to approximate the solutions of (1) in weighted  $L^P$  spaces by a “modified” Nyström method using the Gauss-Jacobi quadrature rule.

The stability and the convergence of the proposed method are proved in weighted  $L^2$  spaces and error estimates are given.

Moreover, in order to show the effectiveness of the method, we present some numerical tests.

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## A NYSTRÖM METHOD FOR MIXED BOUNDARY VALUE PROBLEMS ON DOMAINS WITH CORNERS

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In this talk we propose a new numerical method to solve the mixed Dirichlet-Neumann boundary value problem for the Laplace equation

$$\begin{cases} \Delta u(P) = 0, & P \in D \\ u(P) = f_D(P), & P \in \Sigma_D \\ \frac{\partial u(P)}{\partial n_P} = f_N(P), & P \in \Sigma_N \end{cases}$$

where  $D$  is a simply connected bounded region in the plane with a piecewise smooth-boundary  $\Sigma = \Sigma_D \cup \Sigma_N$ ,  $f_D$  and  $f_N$  are given functions on  $\Sigma_D$  and  $\Sigma_N$ , respectively and  $n_P$  is the inner normal vector to  $\Sigma_N$  at  $P$ .

Following a well-known theory, we represent the solution  $u$  as the single layer potential

$$u(A) = \int_{\Sigma} \Psi(Q) \log |A - Q| d\Sigma_Q, \quad A \in D$$

where  $\Psi$  denotes the single layer density function which is the solution of the following system

$$\begin{cases} \int_{\Sigma} \Psi(Q) \log |P - Q| d\Sigma_Q = f_D(P), & P \in \Sigma_D \\ \pi \Psi(P) + \int_{\Sigma} \Psi(Q) \frac{\partial}{\partial n_P} \log |P - Q| d\Sigma_Q = f_N(P), & P \in \Sigma_N. \end{cases}$$

The above system is characterized by a boundary integral equation of the second kind having a Mellin-type integral operator. Hence, for its numerical treatment, we propose a method of Nyström type based on Legendre quadrature formulas which are “modified” around the corners.

We examine the stability of the proposed method, discuss the convergence, which is accelerated by means of regularized technique, and, finally, provide numerical tests showing the efficiency of the new approach.

## SPECTRAL METHODS FOR DISTRIBUTED-ORDER SPACE RIESZ DIFFUSION EQUATIONS

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The Riesz space fractional diffusion equation with distributed order may be written as:

$$\frac{\partial u(x, t)}{\partial t} = \int_1^2 c(\alpha) \frac{\partial^\alpha u(x, t)}{\partial |x|^\alpha} d\alpha + f(x, t, u(x, t)), \quad 0 < t \leq T, \quad 0 < x < L, \quad (1)$$

where  $c(\alpha)$  acting as weight for the order of differentiation is such that ([1], [2])  $c(\alpha) \geq 0$  and  $\int_1^2 c(\alpha) d\alpha = C > 0$  and where  $\frac{\partial^\alpha u(x, t)}{\partial |x|^\alpha}$  is the fractional Riesz derivative given by:

$$\frac{\partial^\alpha u(x, t)}{\partial |x|^\alpha} = \begin{cases} r_\alpha ({}_0D_x^\alpha + {}_xD_L^\alpha) u(x, t), & 1 < \alpha < 2 \\ \frac{\partial^2 u(x, t)}{\partial x^2} & \alpha = 2, \end{cases} \quad (2)$$

where  $r_\alpha = -\frac{1}{2 \cos(\frac{\pi\alpha}{2})}$ ,  $\alpha \neq 1$ , and  ${}_0D_x^\alpha$  and  ${}_xD_L^\alpha$  are the left-sided and right-sided Riemann-Liouville derivatives, respectively, defined by:

$${}_0D_x^\alpha u(x, t) = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_0^x (x-s)^{1-\alpha} u(s, t) ds$$

$${}_xD_L^\alpha u(x, t) = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_x^L (s-x)^{1-\alpha} u(s, t) ds.$$

Here we will be concerned with the numerical solution of this class of equations. We describe a Chebyshev collocation method to approximate the solution of (1) subject to an initial condition and two Dirichlet-type boundary conditions. Some numerical examples are provided for discussion and comparison.

This is a joint work with Neville Ford from Chester University, M. Luisa Morgado from University of Trás-os-Montes e Alto Douro and Magda Rebelo from New University of Lisbon.

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## COMPOSED MULTISTEP METHODS FOR ODES

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Modified extended backward differentiation formulae (MEBDF) were introduced by Cash [1]. This class of methods is suitable for the numerical integration of first order systems of stiff ordinary differential equations. In this work we take advantage of the framework of General Linear Methods to introduce the class of Composed Multistep (CM) methods in order to analyze and to improve the stability properties of MEBDF methods and of Perturbed MEBDF methods introduced in [2]. Example of  $A$ -stable CM methods are provided up to order  $p = 6$ , and CM methods with large angle of  $A(\alpha)$ -stability are constructed for  $p > 6$ . Numerical experiments which confirm the good performance of these methods are also reported. (This is a joint work with Zdzislaw Jackiewicz).

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# A PRODUCT INTEGRATION METHOD FOR NONLINEAR FREDHOLM INTEGRAL EQUATIONS IN L1

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We consider a weakly singular Fredholm integral operator  $T : X \rightarrow X$  defined by

$$(Tx)(s) = \int_a^b H(s, t)L(s, t)N(x(t))dt.$$

where the functions  $(s, t) \rightarrow L(s, t)$  and  $s \rightarrow N(s)$  are regular and  $(s, t) \rightarrow H(s, t)$  is weakly singular function. Our aim is to find an approximation of the solution in  $X = L^1([a, b])$  of the equation

$$(T - z)\varphi = y.$$

In a previous paper we adapted the product integration method in  $L^1([a, b])$  for linear Fredholm integral equations of the second kind. Our purpose is to extend it in the nonlinear framework. So we propose an approximate operator of  $T$  in  $L^1([a, b])$  and then we prove the existence and uniqueness of the approximate solution. Numerical evidence is given.

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## A NUMERICAL METHOD FOR THE SOLUTION OF AN EXTERIOR NEUMMAN PROBLEM ON DOMAINS WITH CORNERS

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In this talk we are concerned with the exterior Neumann problem for the Laplace equation in two-dimensional domains with piecewise smooth boundaries.

Let  $\Omega \subset \mathbb{R}^2$  be an open, bounded simply connected domain, with a piecewise smooth Lipschitz boundary  $\Gamma$ . We shall assume that the boundary curve  $\Gamma$  contains  $r$  corner points  $P_1, \dots, P_r$  and is otherwise smooth. We consider the problem

$$\begin{aligned} \Delta u &= 0, & \text{in } \mathbb{R}^2 \setminus \bar{\Omega}, \\ \frac{\partial u}{\partial n} &= f, & \text{on } \Gamma, \\ |u(x)| &= o(1), & \text{as } |x| \rightarrow \infty, \end{aligned} \quad (1)$$

where  $n$  denotes the unit normal to the boundary  $\Gamma$  directed into the exterior  $\mathbb{R}^2 \setminus \bar{\Omega}$ . We shall assume that the given Neumann data  $f$  is a sufficiently smooth function which satisfies

$$\int_{\Gamma} f ds = 0. \quad (2)$$

A boundary integral equation (BIE) formulation of the exterior Neumann problem (1) is obtained by using the single layer representation of the potential  $u$ , i.e.

$$u(x) = - \int_{\Gamma} \phi(y) \log |x - y| dS(y), \quad x \in \mathbb{R}^2 \setminus \bar{\Omega}, \quad (3)$$

where  $|x - y|$  is the Euclidean distance between  $x$  and  $y$ ,  $dS(y)$  is the element of arc length and  $\phi$  is the so called single-layer density function. The single layer potential (3) is a solution of (1) provided the density  $\phi$  is a solution of the integral equation

$$-\pi\phi(x) - \int_{\Gamma} \frac{\partial}{\partial n(x)} \log |x - y| \phi(y) dS(y) = f(x), \quad x \in \Gamma, \quad (4)$$

and in addition satisfies

$$\int_{\Gamma} \phi(y) dS(y) = 0. \quad (5)$$

By applying a suitable decomposition of the boundary  $\Gamma$ , the BIE (4) can be converted into a system of  $r$  integral equations. A “modified” Nyström type method, based on the Gauss Legendre quadrature rule, is proposed in order to approximate the solution of this system.

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## NUMERICAL APPROXIMATION OF SINGULAR SOLUTIONS OF THE DYNAMIC GINZBURG–LANDAU EQUATIONS

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We study the time-dependent Ginzburg–Landau equations (TDGL) in a polygon, possibly with reentrant corners. After proving well-posedness of the equations and decomposing the solution as a regular part plus a singular part, we see that the magnetic potential is not in  $H^1(\Omega)$  in general, and so the standard finite element method (FEM) may give incorrect solutions. To overcome this difficulty, we reformulate the equations into an equivalent system of elliptic and parabolic equations based on the Hodge decomposition, which avoids direct calculation of the magnetic potential. The essential unknowns of the reformulated system admit  $H^1$  solutions and can be solved correctly by the FEMs. We then propose a decoupled and linearized FEM to solve the reformulated equations and present error estimates based on the proved regularity of the solution. Numerical examples are provided to support our theoretical analysis and show the efficiency of the method.

## **ON THE CONVERGENCE OF A FINITE DIFFERENCE SCHEME FOR A SECOND ORDER DIFFERENTIAL EQUATION CONTAINING NONLINEARLY A FIRST DERIVATIVE**

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This work is concerned with the convergence of a finite difference scheme to the solution of a second order ordinary differential equation with the right-hand-side nonlinearly dependent on the first derivative. By defining stability as the linear growth of the elements of a certain matrix and combining this with consistency, convergence is demonstrated. The stability concept is then interpreted in terms of a root condition.

## AN EDGE DETECTION METHOD FOR METAL GRAIN VIA A REACTION DIFFUSION SYSTEM

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**Abstract** Prior austenite grain size (PAGS) is an important parameter in the high-carbon high chromium steel. After the quenching and tempered, this type of steel consisted of martensite block and packet which were strongly related to PAGS. We need a computer tool to calculate this parameter to process a large number of images. Because the grain boundary is not so clear, automatic detection of edges of grain is not easy. Here, we propose a new image analyzing method to detect the grain boundary via a reaction diffusion system. We will introduce this method and show some numerical results.

### Introduction

Our research group has investigated PAGS control and used the repeated heating which has been one of the PAGS refinement methods. We have several results related to the PAGS; rotating bending fatigue [3], rolling contact fatigue [10] and reciprocating wear [2]. Based on these results, we applied the homology method to steel structures analysis [5] and classified three sizes of repeatedly quenched PAGs [6]. The homology method has been developed to detect the cancer area from the digital images [7] and [8]. To apply the this method, we have to get the grain boundary from the microstructure image, clearly. The boundary is, however, not always clear. We have needed to trace the prior austenite grain lines by our own hands.

In this study, we developed a new image analyzing method by using a reaction diffusion system. Because this method can be applied several kinds of images, we will introduce not only the images of prior austenite grain but also the image of the capillary vessels. In order to evaluate the effectiveness of this method, we compared between this reaction diffusion method and the clear grain image of handwriting.

### The reaction diffusion system

The reaction diffusion system is often used to analyze self-organization phenomenon. Here, we apply this system to detect the vaguely grain boundary. This idea was developed by Nomura et al (cf. [9]) for detecting the edges in the image that has variations in the brightness [9]. First, a local average threshold is determined by a diffusion equation as follows:

$$\frac{\partial a}{\partial t} = D_a \nabla^2 a \quad (1)$$

where  $D_a$  is the diffusion coefficient. The valuable  $a$  is a threshold for firing of the following Fitz-

Hugh Nagumo equations (3) and (4) (cf. [1, 4]). The initial value  $a_0$  of  $a$  is determined by

$$a_0 = 0.15 + 0.2 \frac{I - I_{min}}{I_{max} - I_{min}} \quad (2)$$

where  $I$  is the brightness of pixels with the gray scale (0 - 255) in the original image,  $I_{max}$  and  $I_{min}$  are maximum and minimum brightness value of pixels. Next, a reaction-diffusion system with the Fitz-Hugh Nagumo equation (FHN) is used. The system is described as

$$\frac{\partial u}{\partial t} = \frac{1}{\varepsilon} [u(1-u)(u-a) - v] + D_u \nabla^2 u \quad (3)$$

$$\frac{\partial v}{\partial t} = u - bv + D_v \nabla^2 v \quad (4)$$

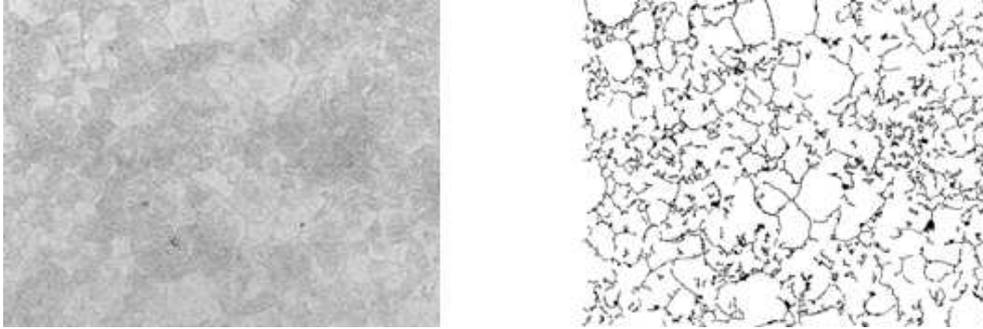
where  $D_u$  and  $D_v$  are diffusion coefficients for the variables  $u$  and  $v$ , the parameter  $\varepsilon$  is a positive small constant ( $0 < \varepsilon \ll 1$ ).  $b$  is a positive constant and spatially homogeneous. The initial value of  $u$  is set as

$$u_0 = 0.15 + (C - 0.15) \frac{I - I_{min}}{I_{max} - I_{min}} \quad (5)$$

where  $C$  is a constant parameter and appropriate value of this parameter depends on the original image for edge detection. The initial value  $v = 0$  homogeneously.

## Results and discussions

Figure 1 (a) shows a prior austenite grain structure whose area is  $5.9 \cdot 10^4 \mu m^2$ . These specimens were etched by picral and the black lines represent the PAG boundaries. Figure 1 (b) shows the our numerical result.



(a) (b)

Figure 1 (a) a prior austenite grain structure whose area is  $5.9 \cdot 10^4 \mu m^2$ .  
(b) shows the our numerical result.

We can emphasize the vague boundary of the grain by using our method. However, the result is not sufficient to the engineering demands. By combining another method, we need to detect the edge more clearly. We will introduce the idea, too.

## Conclusion

We developed a new edge detecting method by using a reaction diffusion system. In this study, we prepared quenched high-carbon, high-chromium steel samples (JIS-SUJ2). It has a great potential as a method of image processing from the row microstructure image. We can apply this method not only extracting the grain boundaries but also the image of capillary vessels.

## Acknowledgement

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## APPROXIMATION OF HADAMARD FINITE PART TRANSFORMS ON $(0, +\infty)$

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This talk deals with the numerical approximation of *Hadamard Finite Part Transforms* of the type

$$\mathbf{H}_p(fw_\alpha, t) = \int_0^{+\infty} \frac{f(x)}{(x-t)^{p+1}} w_\alpha(x) dx, \quad w_\alpha(x) = e^{-x} x^\alpha, \quad (1)$$

where  $p \geq 1$  is integer and  $t > 0$ .

This kind of integral transforms were introduced in [3] and are employed in the numerical solution of hypersingular integral equations, often models for physics and engineering problems (see [5] [4], [2]). In particular, FP integrals reducible to the type (1) are involved in the solution of hypersingular integral equations coming from Neumann 2D elliptic problems on semiplanes by using a Petrov-Galerkin infinite BEM approach [1]. Recently in [6] we have proposed a numerical method useful for approximating integrals of the type (1) for any fixed  $t$ . Here we propose a procedure for the approximation of the function  $\mathbf{H}_p(fw_\alpha, t)$ . To be more precise, setting

$$\begin{aligned} \mathbf{H}_p(fw_\alpha, t) &= \int_0^{+\infty} \frac{f(x) - \sum_{k=0}^p \frac{f^{(k)}(t)}{k!} (x-t)^k}{(x-t)^{p+1}} w_\alpha(x) dx \\ &+ \sum_{k=0}^p \frac{f^{(k)}(t)}{k!} \int_0^{+\infty} \frac{w_\alpha(x)}{(x-t)^{p+1-k}} dx \\ &=: \mathbf{F}_p(f, t) + \sum_{k=0}^p \frac{f^{(k)}(t)}{k!} \mathbf{H}_{p-k}(w_\alpha, t), \end{aligned}$$

we approximate the function  $\mathbf{F}_p(f)$  by means of the  $p$ -th derivative of a suitable Truncated Lagrange polynomial [8] interpolating  $\mathbf{F}_0(f, t)$  at the zeros of the  $m$ -th Laguerre polynomial  $p_m(w_\alpha)$  (see [9]). The procedure employs the Truncated Gauss-Laguerre rule [7], by exploiting the "good" distance between the zeros of the Laguerre polynomials. Since using the same values of the function  $f$  we approximate also  $\{f^{(k)}(t)\}_{k=1}^p$  by a simultaneous approximation process, all the computation of  $\mathbf{H}_p(f, t)$  can be performed without computing the derivatives of  $f$ .

The convergence and stability of the method are proved in suitable weighted spaces of continuous functions. Some numerical tests confirming our theoretical estimates are proposed.

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# EVOLVING RADIAL BASIS FUNCTION NEURAL NETWORK: A LEARNING ALGORITHM FOR TIME SERIES FORECASTING

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Radial basis function neural networks were introduced by Broomhead and Lowe in [1], being their main applications regression problem and time-series forecasting, as well as classification or clustering tasks. They have remarkable properties such as localization, functional approximation, interpolation and cluster modeling. Applying RBF in approximation theory shows optimal properties [2, 3, 4, 5]. They have been shown to model any continuous input-output mapping and to provide a simple model for complex networks. RBF neural networks are thought as a two-layer, feed-forward network in which hidden neuron activation functions are RBFs.

Let  $\Omega$  be a nonempty set, a *multivariate* function

$$K : \Omega \times \Omega \rightarrow \mathbb{R}$$

is called radial, so that it can be presented via a *univariate* function  $\phi : [0, \infty) \rightarrow \mathbb{R}$

$$K(x_i, x_j^c) = \phi(\|x_i - x_j^c\|).$$

RBFs are positive definite symmetric function on  $\Omega$ . The RBF  $K(x_i, x_j^c)$  reaches its optimum on center point  $x_i^c$ , and decreases/increases to sample value far from  $x_i^c$ . The radius,  $r$ , controls the increment or decrements of likelihood regarding to the center.

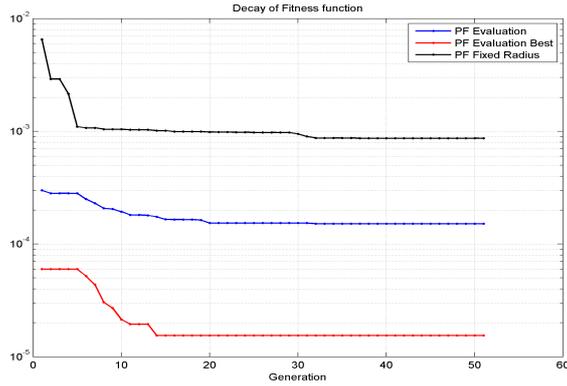
The main difficulties in RBFNNs concerned the choice of center points and the scale of the basis in order to best fit;

1. **Selection of the center points (number and value):** the number of the hidden neurons critically affects the results. In traditional regularization RBF, the number of basis equals the number of the training set. Although with many hidden neurons we get the well results, but the result model will not be a powerful model for prediction applications. This is so-called overfitting problem. Which is also complex and often ill-conditioned [6]. In other hand, not sufficient hidden neurons can simply cause poor approximation results.
2. **Selection of the radius:** the small value of the radius can lead to overfitting. The very wider radius can affects the efficiency of the data information and lead to the worst results [7].

These leads to singularities problem in the parameters( centers and radius) space.

In this research we apply some evolutionary algorithms to train the parameters. The evolutionary algorithms are stochastic algorithms (not deterministic), that are based on natural evolution. In principle, this is based on the "survival" of the "fittest". The exploration and the exploitation part of algorithm is due to the selection process.

After certain generation the process of learning does not have efficient improvements. The singular regions of parameters space cause this plateau. Figure (1) shows this phenomena in learning process based on Genetic algorithm with various loss functions.



**Figure 1.** Decay of error functions with scaled radius and constant radius . Red line depicts the Best result from error functions with scaled radius, once the testing iteration done.

This paper focuses on elimination singularities in RBFNN based on different heuristic algorithms. We apply the *scaled RBFs* for model. One proper search algorithm can explore the good parameters to reduce the error. We implement the Algorithms on time series modeling/forecasting.

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## NUMERICAL SOLUTION OF FRACTIONAL INTEGRO-DIFFERENTIAL EQUATIONS

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The numerical solution of fractional integro-differential equations involving Caputo-type fractional derivatives is discussed. Using an integral equation reformulation of the corresponding initial or boundary value problem, first some regularity properties of the exact solution are derived. Based on these properties and spline collocation techniques, the attainable order of convergence of the proposed algorithms is studied, theoretically and numerically. Our approach is based on some ideas and results of [1, 2, 3].

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## ANALYTICAL AND CONSTRUCTIVE APPROACH TO IMPULSIVE BOUNDARY VALUE PROBLEMS

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We investigate the boundary value problem

$$x'(t) = f(t, x(t)) \text{ for a.e. } t \in [a, b], \quad \ell(x) = c \in \mathbb{R}^n, \quad (1)$$

with a linear and bounded operator  $\ell$ .

First, under the assumption that  $f$  is the Carathéodory function and that the boundary value problem (1) is subject to the state-dependent impulse conditions

$$x(t+) - x(t-) = J_i(x(t-)) \text{ for } t \in (a, b) \text{ such that } t = \gamma_i(x(t-)), \quad (2)$$

where  $J_i$  and  $\gamma_i$  are continuous,  $i = 1, \dots, p$ ,  $p \in \mathbb{N}$ , we use an analytical approach and derive a general existence principle. The principle serve as a tool for the proofs of the solvability of the impulsive boundary value problem (1), (2) with various data functions  $f$ ,  $J_i$ ,  $\gamma_i$  and  $\ell$ , see e.g. [1].

Then we consider problem (1) with  $f$  continuous and with the state-dependent impulse condition

$$x(t+) - x(t-) = J(x(t-)) \text{ for } t \in (a, b) \text{ such that } g(t, x(t-)) = 0. \quad (3)$$

For the impulsive boundary value problem (1), (3) a constructive approach is used, and conditions which allow to realize a construction of a solution are presented. Proofs and illustrative examples can be found in [2].

Let us note that the impulse instants  $t \in (a, b)$  in (2) or in (3) are state-dependent which means that they are not known before and depend on a solution  $x$ .

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## INTRODUCING DELAY DYNAMICS TO BERTALANFFY'S SPHERICAL TUMOUR GROWTH MODEL

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We introduce delay dynamics to von Bertalanffy's ordinary differential equation model of tumour growth

$$x'(t) = \alpha x^{\frac{2}{3}}(t - \tau_1) - \beta x(t - \tau_2), \quad (1)$$

a model which has received little attention in comparison to other models, such as the Gompertz, Greenspan and Logistic models. Through parameter estimation and the use of existing, historical data, we demonstrate its potential suitability for modelling the growth of spherically-shaped tumours. The nature of the nonlinear term leaves us resorting to fixed point theory in order to establish some qualitative results about the solution of the equation.

This work was conducted jointly with Dr Asmaa Al Themairi, Department of Mathematical Science, University of Princess Nourah bint Abdulrahman, Saudi Arabia, [aialthumairi@pnu.edu.sa](mailto:aialthumairi@pnu.edu.sa).

## NYSTRÖM METHODS FOR FREDHOLM INTEGRAL EQUATIONS DEFINED ON STRIPS

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We investigate the numerical solution of two-dimensional Fredholm integral equations defined on a strip of the type  $S = (-\infty, +\infty) \times [-1, 1]$ ,

$$f(x, y) - \mu \int_S k(x, y, s, t) f(s, t) \mathbf{w}(s, t) ds dt = g(x, y), \quad (x, y) \in S,$$

where  $\mathbf{w}(x, y) := w_1(x)w_2(y)$  and  $w_1(x) = |x|^\gamma e^{-x^2}$ ,  $w_2(y) = (1 - y)^\alpha(1 + y)^\beta$ ,  $\alpha, \beta, \gamma > -1$ , are suitable weight functions of Generalized Hermite and Jacobi type respectively,  $\mu$  is a real number.  $k$  and  $g$  are given functions defined on  $((-\infty, +\infty) \times [-1, 1])^2$  and  $(-\infty, +\infty) \times [-1, 1]$  respectively,  $f$  is the unknown function.

The known functions will be considered to be sufficiently smooth on the open sets, but they, or their derivatives, could have (algebraic) singularities on the finite boundaries and/or on the segment  $x = 0$ . Moreover they are allowed to have an exponential growth at  $\pm\infty$  at most.

We will study the solvability of the equation in spaces of functions defined on  $S$  and equipped with a suitable weighted uniform norm.

Then we introduce some Nyström methods based on cubature formulas obtained as a tensor product of two Gaussian quadrature formulas w.r.t. the weights  $w_1, w_2$ . Due to the “unboundedness” of the domain we will need “truncated” cubature rules. The convergence, stability and well conditioning of the methods are proved in the weighted spaces of functions mentioned before. Some numerical examples will illustrate the efficiency of the methods.

# OPTICAL FLOW WITH FRACTIONAL ORDER REGULARIZATION: VARIATIONAL MODEL AND SOLUTION METHOD

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Optical flow is a tool for detecting and analyzing motion in a sequence of images. The underlying idea is to depict the displacement of patterns in the image sequence as a vector field, named the optical flow vector field, generating the corresponding displacement function. In their seminal paper, Horn and Schunck [2] proposed a variational method for the computation of the optical flow vector field. In this approach an energy functional is minimized consisting of a similarity term (or data term) and a regularity term:  $\operatorname{argmin}_{u \in \mathcal{H}} E(u) = \operatorname{argmin}_{u \in \mathcal{H}} (\mathcal{S}(u) + \mathcal{R}(u))$ . The space  $\mathcal{H}$  denotes an admissible space of vector fields,  $\mathcal{R}$  denotes the regularity term for the vector field  $u$ , and  $\mathcal{S}$  denotes the similarity term, which depends on the image sequence  $I$  under consideration. To overcome some of the difficulties presented by the Horn-Schunck functional, several extensions and improvements have been developed [5]. To obtain robust and discontinuity preserving solutions for optical flow, in [6] a modification of the classical model is proposed, which consists in considering an  $L1$  norm in the regularizing term and the similarity term is substantially changed by introducing an auxiliary variable  $v$ .

In this work we present an optical flow model for a sequence of images defined on a domain in  $\mathbb{R}^2$  which consists of a modification of the model introduced in [6], by considering for the regularization term the  $L1$  norm of a fractional derivative operator [1]. The numerical method developed to solve the minimization problem involves the Split Bregman method described in [3]. The effectiveness of the new model and numerical approach is shown by presenting the experimental results obtained when we use the test sequences available in the Middlebury benchmark database designed by [4] and by comparing its performance with other existing numerical methods.

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## COMPUTATIONAL METHODS FOR A FORWARD-BACKWARD EQUATION FROM PHYSIOLOGY

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It is presented a numerical scheme which approximates the solution of a particular non-linear mixed type functional differential equation from physiology, adapted from the work introduced in [1, 2, 3]. The mathematical equation models a superficial wave propagating through the tissues. Two different approximations of considered equation are taken into account when it is assumed a small time delay or an arbitrary time delay.

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# MODIFICATION OF THE NONLINEAR SCHRÖDINGER EQUATION AS A MODEL OF PROPAGATION OF ELECTROMAGNETIC WAVES IN NANOSTRUCTURES

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In this work a modification of the Nonlinear Schrödinger Equation (NLS) in nanostructures is considered. The dielectric permittivity depends on the electric vector, the number of molecules of nanosystem and the current coordinate. The modification of the NLS for the function  $\psi$  (which is used to determine the electric and magnetic vector) can be written in the following form:

$$\frac{\partial^2 \psi}{\partial z^2} + i \frac{\partial \psi}{\partial r} + i \frac{\psi}{2r} \pm |\psi|^2 f(r) \psi = 0, \quad (1)$$

where the function  $f(r)$  depends on the optical properties of the system. The given equation corresponds to the cylindrical model of system. At  $f(r) = 1$  the substitution from paper [1] transforms it to the classical NLS. The equation (1) with different functions  $f_i(r)$  can describe the propagation of electromagnetic waves in complex mezo- and nanosystems. The equation (1) is a singular equation when the point  $r = 0$  belongs to the system. In the general case a singularity can arise in other points determined by the function  $f(r)$ . The solution was carried out with the help the substitution from paper [1] and numerical methods. The influence of the geometric characteristics of the system on the value of  $\psi$  was investigated. The modification of the equation (1) for longitudinal electromagnetic waves was also considered.

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## A MESHFREE METHOD FOR HARMONIC PROBLEMS WITH SINGULAR BOUNDARY CONDITIONS

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The method of fundamental solutions (MFS) is a meshfree and integration free boundary collocation method, initially developed in the 1960's for the numerical solution of elliptic boundary value problems, e.g. [1, 2]. In recent decades, MFS has become increasingly popular among the scientific community due to its simple formulation, low computational cost and high accuracy, when applied to BVPs with analytic boundary conditions, posed in sufficiently regular domains, e.g. [3].

However, due to the analyticity of the shape functions, Gibbs phenomenon occurs in the neighborhood of any boundary condition singularity and the classical MFS fails to converge in non smooth settings. In this talk we present a variant of the MFS which allows us to solve accurately Laplace's PDE coupled with discontinuous Dirichlet type boundary conditions. In order to solve this singular problem we augment the MFS approximation basis with a set of harmonic functions which exhibit the correct singular behavior on the boundary of the domain. We derive such functions, also known as cracklets [4, 5], by analytic evaluation of the double layer potential for the polynomial canonical basis

$$\Psi_i(x) = \int_{\Gamma} \partial_{\nu_y} \Phi(x-y) y^i ds_y, \quad x \in \Omega \subset \mathbb{R}^2, \quad i = 0, 1, 2, \dots,$$

where  $\Gamma \subset \partial\Omega$  is a reference line segment, depending on the location of the singularity,  $\Phi$  is the fundamental solution to the Laplace operator and  $\nu_y$  is the exterior normal unitary vector at  $y \in \Gamma$ .

This new approach may be viewed as a hybrid method, resulting from the coupling between a BEM approximation to the singular part of the solution and a MFS approximation to its regular part, without explicitly splitting the total solution into two parts. The meshfree characteristics of the method are also preserved and the total approximate solution of the BVP is calculated by solving, in the least squares sense, a collocation linear system.

The performance of the proposed method will be illustrated for several 2D interior boundary value problems and different boundary conditions.

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## HIERARCHICAL MATRICES ON THE EIGENVALUE COMPUTATION OF INTEGRAL OPERATORS

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We consider the numerical solution of a large eigenvalue problem resulting from a finite rank discretization of an integral operator. We are interested in computing a few eigenpairs, with an iterative method, so a matrix representation that allows for fast matrix-vector products is required. Hierarchical matrices are appropriate for this setting, and also provide cheap LU decompositions required in the spectral transformation technique. We illustrate the use of freely available software tools to address the problem, in particular SLEPc for the eigensolvers and HLib for the construction of  $\mathcal{H}$ -matrices. We develop analytical expressions for the approximate degenerate kernels and deduce error upper bounds for these approximations. Numerical tests show the benefits of the data-sparse representation compared to standard storage schemes, in terms of computational cost as well as memory requirements.

This work was done with the collaboration of A. L. Nunes, J. E. Roman and M. Ahues ([1], [2]).

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### 3. THIRD PART: ABSTRACTS OF THE POSTERS PRESENTATIONS

## POSTERS



## HIGH ORDER EXPONENTIALLY FITTED METHODS FOR PERIODIC VOLTERRA INTEGRAL EQUATIONS

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Volterra integral equations with periodic solution of the type

$$\begin{aligned}y(x) &= f(x) + \int_{-\infty}^x k(x-s)y(s)ds, & x \in [0, x_{end}], \\y(x) &= \psi(x), & -\infty < x \leq 0,\end{aligned}$$

model a number of periodic phenomena with memory, e.g. the spread of seasonal epidemics. An efficient and accurate numerical solution of these equations may be found by means of special purpose methods, which exploit the a priori knowledge of the qualitative behavior of the solution. On this direction, we propose exponentially-fitted direct quadrature methods of high order. The coefficients of these methods depend on the frequency of the problem, to reduce the error when periodic problems are treated and an estimate of the frequency is available. In this talk we present the construction and analysis of these methods, and illustrate their performances on some significant test problems.

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## PARALLEL METHODS FOR WEAKLY SINGULAR VOLTERRA INTEGRAL EQUATIONS ON GPUS

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Large systems of weakly singular Volterra Integral Equations (VIEs) arise as mathematical models in several applications, especially in the semi-discretization in space of fractional partial differential equations (PDEs) [6, 7, 8]. It is known that the numerical treatment of large systems of VIEs can be more efficient if carried out in a parallel computational environment. However parallel architectures may be quite expensive. A more reasonable balance between efficient solution and sustained cost can be successfully reached by employing modern hardware devices, such as Graphics Processing Units (GPUs). GPUs were initially designed for computer graphics, but nowadays they are employed as general purpose high-performance parallel processors, due to their cheap cost and their great computational capability [9].

The purpose of this talk is to describe the employ of GPUs for the numerical solution of large systems of VIEs by means of waveform relaxation (WR) methods [1, 2, 3, 4]. A GPU acceleration of WR methods for ordinary differential equations (ODEs) can be found in [5]. WR methods are iterative methods particularly suited to solve large systems of ODEs or VIEs, as they are designed in order to decouple the original large system in smaller subsystems: in this way, the iteration process can be implemented in a parallel computational environment, since each subsystem can be treated by a single processor. This iteration process realizes what is commonly known as *parallelism across the system*. We show the numerical results on large system of VIEs arising from the semi-discretization in space of fractional PDEs, showing the obtained speed-up.

This work has been supported by GNCS-INDAM.

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## ON CORDIAL VOLTERRA INTEGRAL EQUATIONS

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We are concerned with Volterra integral equations of the form

$$\mu u = V_\varphi u + f$$

where

$$(V_\varphi u)(t) = \int_0^t \underbrace{t^{-1}\varphi(s/t)}_{K(t,s)} u(s) ds, \quad t \in [0, T].$$

The operator  $V_\varphi$  is called a cordial Volterra operator and we assume its *core* function  $\varphi$  to be in  $L^1[0, 1]$ . Such operator is noncompact and it satisfies the following properties:

$V_\varphi(t)$  is bounded in  $C[0, T]$ ;

$u_r(t) = t^r$  are eigenfunctions

and  $C_r = \int_0^1 \varphi(s) s^r ds$  are the corresponding eigenvalues.

Examples of kernels which generate such type of operators include

- $K(t, s) = t^{-\alpha} s^{\alpha-1} = t^{-1} \varphi(s/t)$ , with:  $\varphi(x) = x^{\alpha-1}$  ( $\alpha > 0$ ) (heat conduction probl.)
- $K(t, s) = (t^\gamma - s^\gamma)^{-1/\gamma} = t^{-1} \varphi(s/t)$ ,  
with:  $\varphi(x) = (1 - x^\gamma)^{-1/\gamma}$  ( $1 < \gamma < \infty$ ). (due to Lighthil, for  $\gamma = 3/2$ )

In this presentation we will focus on the analytical and numerical properties of such equations. Some results were obtained in collaboration with Gennadi Vainikko.

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## A STOCHASTIC APPROACH TO NEURAL FIELD EQUATIONS ON UNBOUNDED DOMAINS

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Neural Field Equations (NFE) are a powerful tool for analysing the dynamical behaviour of populations of neurons. The analysis of such dynamical mechanisms is crucially important for understanding a wide range of neurobiological phenomena. As in other sciences, in Neurobiology it is well-known that better consistency with some phenomena can be provided if the effects of random processes in the system are taken into account. In the recent work of Kühn and Riedler [1], the authors study the effect of additive noise in Neural Field Equations. With this purpose they introduce the stochastic integrodifferential equation

$$dU_t(x) = \left( I(x, t) - \frac{1}{c}U_t(x) + \int_{\Omega} K(|x - y|)S(U_t(y))dy \right) dt + \epsilon dW_t(x), \quad (1)$$

where  $t \in [0, T]$ ,  $x \in \Omega \subset \mathbb{R}^n$ ,  $W_t$  is a Q-Wiener process.

The main goal of the present work is to analyse the effect of noise in certain neural fields with delay, which are known to have Hopf bifurcations. In this case we consider the following modification of equation (1)

$$dU_t(x) = \left( I(x, t) - \frac{1}{c}U_t(x) + \int_{\Omega} K(|x - y|)S(U_{t-\tau}(y))dy \right) dt + \epsilon dW_t(x), \quad (2)$$

where, as in the deterministic case,  $\tau$  is a delay, depending on the distance  $|x - y|$ . Equation (2) is completed with an initial condition of the form

$$U_t(x) = U_0(x, t), \quad t \in [-\tau_{max}, 0], \quad x \in \Omega, \quad (3)$$

where  $U_0(x, t)$  is some given stochastic process,  $\tau_{max}$  is the maximum value of the delay. In our case,  $\Omega = \mathbb{R}$ .

In order to approximate equation (2) we apply a numerical scheme which uses the Galerkin method for the space discretization. In this way we obtain a system of stochastic delay differential equations, which are then discretized by the Euler-Maruyama method.

We use this computational algorithm to analyse noise induced changes in the dynamical behaviour of some neural fields. Some numerical examples are presented and the results are discussed.

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## COLLOCATION METHODS WITH SMOOTHING VARIABLE SUBSTITUTIONS FOR SINGULAR $M$ -LAPLACIAN FREE BOUNDARY PROBLEMS

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Many mathematical models in Physics and Mechanics lead to the following free boundary problem: find a real  $M > 0$  and a positive solution of the equation

$$(|y'|^{m-2} y')' + \frac{N-1}{x} |y'|^{m-2} y' + f(y) = 0, \quad 0 < x < M, \quad (1)$$

which belongs to  $C^2((0, M)) \cup C^1([0, M])$  and satisfies the boundary conditions

$$y'(0) = 0, \quad y(M) = y'(M) = 0, \quad M > 0. \quad (2)$$

Concerning the parameters in (1),  $N$  is the space dimension ( $N \geq 2$ ),  $m > 1$  and

$$f(y) = ay^q - by^p, \quad (3)$$

where  $p < q$  and  $a, b > 0$ .

Based on the results in [2], where smoothing variable transformations were proposed to deal with the singularities at  $x = 0$  and  $x = M$ , here we transform the free boundary problem into an eigenvalue problem. By applying to the resulting equations the smoothing variable transformations we obtain a new problem, which we solve using the open domain MATLAB code `bvpsuite` [1]. Several numerical results are presented and discussed.

This is a joint work with Pedro M. Lima (CEMAT, University of Lisbon), S. Schirnhoffer, M. Schöbinger and E. Weinmüller (Vienna University of Technology, Austria).

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# THE APPLICATION OF HOMOLOGY ANALYSIS FOR THE PERIODIC PATTERNS

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Image analysis methods are one of the strongest tools to estimate the properties of the materials. Speeding up of computers supports this method. Common methods for estimation the pattern are measuring the area and the perimeter length, particle analysis, Fast Fourier Transform, and so on. These methods estimate some of the features of the image. However, to estimate the geometrical properties is difficult by these methods. In this paper, we apply the homology analysis to estimate the geometrical properties of periodical patterns. Two similar patterns (spiral and target patterns) were analyzed by the homology analysis. Our trial showed clear differences between the homology parameters of spiral and target patterns. Namely, our results indicated that the Homology analysis is one of the strongest tools for estimation of geometrical properties.

## Introduction

Biological systems exhibit variety of ordered pattern, e.g., stripe and/or dot pattern on animal skin[3], spiral pattern formed by true slime mold [1], and an action potential and/or Ca<sup>2+</sup> wave travelling on cardiac muscle [4]. The researchers have reproduced those patterns using non-living model systems and uncovered the mechanism of the pattern formation processes to understand the essence of such interesting biological phenomena. One of the most important points are how to analyze the pattern formulation. Estimation of the patterns, quantitatively, is necessary to compare the patterns formed in biological and non-living systems. Usually, ordered patterns are analyzed by Fast Fourier Transform (FFT), which tells us the period and symmetric property of the ordered pattern. However, FFT is not suitable to analyze noisy pattern or disordered pattern or to get information about topological property of pattern, e.g., difference between target and spiral pattern.

Homology analysis has been received attention in recent years for quantitative estimation of non-periodical structures. Homology gives us information about topological properties. Thus, this method can be applied for non-periodical disordered structures. Indeed, there are recent works about the application of the homology analysis for diagnostic imaging for cancer cell [5] and metallic alloy [6]. Both structures have neither periodicity nor regularity. So, common image analysis method such FFT cannot show the essence of those structures. These examples indicate the homology analysis is suitable method to estimate disordered patterns. For an ordered pattern, the period of the pattern is one of the most important information. In addition to the period, the topological property is also important. For example, FFT analysis is not suitable to distinguish spiral and target pattern with same wavelength. Both patterns are isotropic structure and show same power spectra. Here, we show a usability of the homology analysis to estimate such a topological property and to distinguish those ordered patterns. The targets of our investigation are periodic ordered patterns formed by Belousov-Zhabotinsky (BZ) reaction [2]. In the system, several periodic patterns are formed. We will show that the homology analysis can separate similar patterns appeared in the same systems.

## Results and discussion

Spiral pattern and target pattern with single core were analyzed with two methods (FFT and Homology analysis). Both images of spiral and target patterns were isotropic and had comparable wavelength. So, similar results were obtained by FFT (Fig. 1a-ii, 1b-ii). Although the FFT obtained by the target pattern clearly showed higher ordered signals (Fig. 1b-ii), it originated from highly periodicity of the original pattern and did not indicate the geometrical difference. On the other hand, the homology analysis clearly exhibited difference between spiral and target pattern (Fig. 1a-iv, 1b-iv). With change in the threshold value for binary images, the first parameter decreased for both patterns and reached equilibrium value, while the second parameter showed difference manner between spiral and target patterns. For the spiral pattern, the second parameter was kept 0 up to 160 as the threshold value (Fig. 1a-iv), while the second parameter was 0 up to 110 and increased to the equilibrium value over 150 as the threshold value (Fig. 1b-iv). The binary images indicated that the threshold value from 140 to 160 was suitable to reflect the original pattern (Fig. 1a-iii, 1b-iii). For over 160, the binary image of spiral wave connected, as the results the second value increased. These results indicated that the Homology analysis is suitable for estimation of geometrical properties of pattern such as spiral and target pattern. In the case of 160 as the threshold value, the second parameter of the spiral pattern becomes 0, while the target pattern has nonzero second parameter. This result is reasonable to understand the shape of the pattern. The single core spiral pattern consisted of only single chemical wave. Therefore, the connected component (the second parameter) was 0. On the other hand, the target pattern was composed of a series of concentric circles of chemical waves. Thus, the connected component was nonzero value in the target pattern.

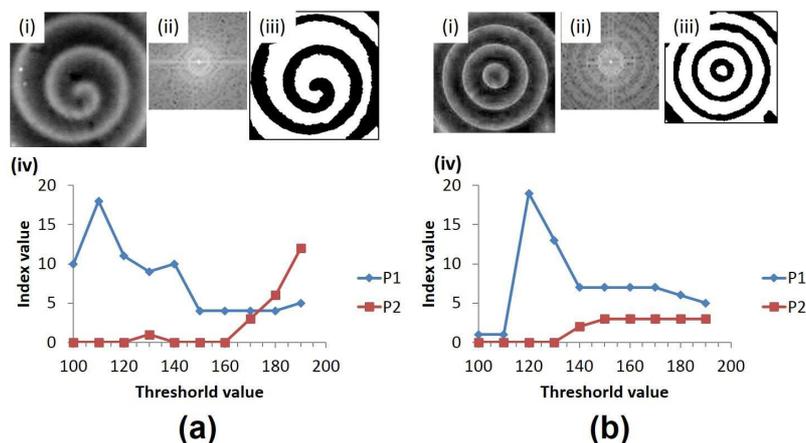


Figure 1. Image analysis results for (a) spiral pattern and (b) target pattern. (i) The original image, (ii) the result of 2D FFT, (iii) the binary images with the threshold value of 160, and (iv) the results of Homology analysis with change in the threshold value.

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## A SPECTRAL COLLOCATION METHOD FOR THE DIFFUSION EQUATION WITH DISTRIBUTED ORDER IN TIME

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In this work we are concerned with the numerical approximation of the reaction-wave diffusion equation with distributed order in time:

$$\int_a^b c(\alpha) \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} d\alpha = \frac{\partial^2 u(x, t)}{\partial x^2} + f(x, t, u(x, t)), \quad t \in (0, A], \quad 0 \leq x \leq L, \quad 0 \leq a < b < 2. \quad (1)$$

subject to suitable initial conditions and boundary conditions of Dirichlet type. The fractional derivative is given in the Caputo sense.

In this work we consider a spectral collocation method, to obtain an approximate solution of (1), based on a Chebyshev series expansion of the solution. Several some numerical results are presented and compared with other numerical approaches.

This is joint work with Neville Ford from University of Chester, Luísa Morgado from UTAD - Department of Mathematics, University of Trás-os-Montes e Alto Douro and Luís Ferrás from Institute for Polymers and Composites, University of Minho.

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