SPECIAL SESIONS

6th Iberian Mathematical Meeting

S2

Applied Partial Differential Equations in Fluids and Materials

Thu 6th, 17:00 - 17:25, Aula 8 – D. Castaño:
Effects of ambient rotation and temperature gradients on the development of a single or double-celled vortex and multiple vortices

Thu 6th, 18:00 - 18:25, Aula 8 – J. Durany:
Thermodynamical behaviour of polythermal ice sheets by using temperature and enthalpy formulations

Thu 6th, 18:30 - 18:55, Aula 8 – J. Ferreira:
Drug release from viscoelastic polymeric platforms: non-Fickian solvent absorption and Fickian drug desorption

Thu 6th, 19:00 - 19:25, Aula 8 – H. Herrero:
Evolution of secondary whirls in dust devil-like vortices in a route to chaos

Thu 6th, 19:00 - 19:25, Aula 9 – F. Guerrero:
An IMEX-WENO scheme for the equilibrium dispersive model of chromatography

Thu 6th, 19:30 - 19:55, Aula 8 – R. López:
Stability and bifurcation of a capillary fluid on an infinite cylinder

Thu 6th, 19:30 - 19:55, Aula 9 – R. Muñoz:

Analysis of a parabolic-elliptic problem with moving parabolic subdomain through a lagrangian approach

Fri 7th, 11:30 - 11:55, Aula 8 – E. Vázquez Cendón:
A local ADER FV/FE projection method for Navier-Stokes equations with turbulence

Fri 7th, 12:00 - 12:25, Aula 8 – P. de Oliveira:
Viscoelastic biodegradable materials: modelling, mathematical analysis and medical applications

Fri 7th, 12:30 - 12:55, Aula 8 – M. Net:
Continuation of periodic orbits in domains heated by the side

Fri 7th, 13:00 - 13:25, Aula 8 – L. Bandeira:
Quasiconvexity, Rank-One Convexity and the Non-Negativeness of Polynomials

Fri 7th, 13:00 - 13:25, Aula 9 – L. Álvarez:
On the minimization of the urban heat island effect in metropolitan areas

Fri 7th, 16:30 - 16:55, Aula 8 – A.C. Barroso:
Second-order structured deformations: relaxation, integral representation and applications

Fri 7th, 17:30 - 17:55, Aula 8 – J. Matias:
Optimal Design of Fractured Media with Prescribed Macroscopic Strain

Fri 7th, 18:00 - 18:25, Aula 8 – J. Tiago:
Modeling the physiopathology of the vascular system

Fri 7th, 18:30 - 18:55, Aula 8 – R. Rodriguez:
Differential equations subject to uncertainty: some connections between different approaches

Fri 7th, 18:30 - 18:55, Aula 9 – C. Rodriguez:
First results on the modelling of heavy metals phytoremediation

Fri 7th, 19:00 - 19:25, Aula 8 – D. Cao:
Two fractional differential equations in mechanics

Fri 7th, 19:00 - 19:25, Aula 9 – M.E.. Vázquez:
Modelling air pollution due to traffic flow in urban networks

Sat 8th, 9:30 - 9:55, Aula 8 – J.L. Ferrín:
Simulación numérica en la U.P.T. de As Pontes

Sat 8th, 10:00 - 10:25, Aula 8 – M. Rebelo:
A numerical method for the space distributed order Riesz fractional diffusion equation

Sat 8th, 10:30 - 10:55, Aula 8 – Ó. López:
Numerical solution of some Fokker-Planck kinetic equations

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Effects of ambient rotation and temperature gradients on the development of a single or double-celled vortex and multiple vortices

D. Castaño[1], **M. C. Navarro**[2], **H. Herrero**[3]

The generation of single or double-celled vortices and multiple vortices in a cylinder non-homogeneously heated from below in a rotation frame is shown in this talk. In a moderate rotation frame, the increase of thermal gradients is the responsible for the progression from a one-celled vortex, characterized by an updraft at the centerline, to a two-celled vortex, characterized by a central eye. If the thermal gradients continue increasing, the axisymmetric eyed-vortex loses the axisymmetry, the eye displaces from the center and tilts. For larger rotation rates, the axisymmetric single-celled vortex does not progress to a double-celled vortex when the thermal gradients increase, but it becomes into a double vortex. The change in the vortex type is also observed in laboratory tornadoes. In Ref. [1] it is shown the progression, as the swirl ratio increases, of vortex structure from a single cell to a two-cell vortex with a downdraft in the center. Our findings are relevant for their connection with the formation and evolution of some atmospheric vortices. The numerical results have been obtained by direct numerical simulation of the time-dependent Navier-Stokes equations coupled with the heat equation, and the boundary conditions. The equations have been solved using a second-order time-splitting method proposed in Ref. [2], and described and tested in Ref. [3] for a cylindrical configuration. For the spatial discretization a pseudo-spectral method is used, with a Fourier expansion in the azimuthal coordinate ϕ and Chebyshev collocation in r and z.

Keywords: Vortices, Thermoconvective instabilities, Navier-Stokes equations

MSC 2010: 74S25, 76B47

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Thermodynamical behaviour of polythermal ice sheets by using temperature and enthalpy formulations

N. Calvo[1], **J. Durany**[1], **C. Vázquez**[2]

In this work an original enthalpy formulation for the thermal behaviour of polythermal ice sheets is proposed and numerically solved. Although the modelling follows some ideas introduced in [1], nonlinear basal boundary conditions in both cold and temperate regions are also considered, thus including the sliding effects in the frame of a fully coupled shallow ice approximation (SIA) model. Then, the highly nonlinear system of partial differential equations governs three main thermomechanical problems: the upper profile evolution, the ice velocity field and the enthalpy distribution. One of the main novelties of this work comes from the introduction of the Heaviside multivalued operator to take into account the discontinuity of the thermal diffusion function at the cold-temperate transition surface (CTS) free boundary. Moreover, we propose a duality method for maximal monotone operators to solve simultaneously the nonlinear diffusive term and the free boundary. In addition, spatial finite element discretizations and Newton' s method for solving the nonlinear system at each time step are performed. Some numerical simulation examples with real data from Antarctica are presented and illustrate the small differences between the computed results from the enthalpy formulation and the alternative formulation in terms of the temperature [2].

Keywords: Ice sheet models, free boundaries, enthalpy, finite elements, duality methods.

MSC 2010: 86A40, 35R35, 65N60, 49M29

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Drug release from viscoelastic polymeric platforms: non-Fickian solvent absorption and Fickian drug desorption

J. A. Ferreira[1], **M. Grassi**[2], **P. de Oliveira**[3], **G. Romanazzi**[1,4]

We consider a polymeric spherical platform containing a solid dispersed drug that is in contact with a solvent fluid. The solid drug in contact with the solvent fluid dissolves and the Fickian release of dissolved drug takes place. While swelling, a non Fickian sorption of the solvent molecules occurs induced by the effect of the viscoelastic properties of the polymer. The fluid entrance, the drug dissolution and the drug release to an external environment are described by a system of PDE's complemented with an equation for the swelling front, initial and boundary conditions. The model includes the two major factors that govern a swelling process of a polymeric platform within a release medium: the cross link density and the concentration of the external medium. Energy estimates for the mass of solvent fluid, undissolved and dissolved drug in the polymeric platform are established. Numerical simulations that illustrate our theoretical results are also included.

Keywords: Drug release, viscoelastic polymers, non-Fickian diffusion, Fickian diffusion

MSC 2010: 35K55, 65N06

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Evolution of secondary whirls in dust devil-like vortices in a route to chaos

D. Castaño[1], **M. C. Navarro**[1], **H. Herrero**[1]

The appearance, evolution and disappearance of periodic and quasiperiodic dynamics of fluid flows in a cylindrical annulus locally heated from below are analysed using nonlinear simulations. The results reveal a route of the transition from a steady axisymmetric vertical vortex to a chaotic flow. The chaotic flow regime is reached after a sequence of successive supercritical Hopf bifurcations to periodic, quasiperiodic and chaotic flow regimes. A scenario similar to the Ruelle-Takens-Newhouse scenario [3] is verified in this convective flow. In the transition to chaos we find the appearance of subvortices embedded in the primary axisymmetric vortex, flows where the subvortical structure strengthens and weakens, almost disappears before reforming again, leading to a more disorganized flow to a final chaotic regime. Results are remarkable as they connect to observations describing the formation, weakening and virtually disappearence before revival of subvortices in some atmospheric swirls such as dust devils [4]. The numerical results have been obtained by direct simulation of the timedependent governing equations, incompressible Navier-Stokes coupled with a heat equation under Boussinesq approximation. These equations have been solved using the second-order time-splitting method. A pseudo-spectral method is used for the spatial discretization, with a Fourier expansion in the azimuthal coordinate and Chebyshev collocation in the radial and vertical coordinates. These works have been published in [1, 2].

Keywords: natural convection, espectral methods, vertical vortex.

MSC 2010: 74S25, 76B47

Referencias

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An IMEX-WENO scheme for the equilibrium dispersive model of chromatography.

F. Guerrero[1], **P. Mulet**[1], **R. Donat**[1]

The nonlinear equilibrium dispersive model consists of a partial derivative equation in the form of viscous conservation law. The solutions of this type of PDEs may contain very sharp transitions and this is the case in this chromatographic model. We show that a high resolution Weighted Essentially Non Oscillatory (WENO) scheme gives accurate numerical solutions which capture the sharp discontinuities present in the chromatographic fronts. Moreover, since the dispersive term in the model imposes a severe restriction in the time step size, we apply an implicit strategy to handle the parabolic term and an explicit one for the convective term to improve the effciency of the numerical scheme. In addition, we show a series of numerical experiments to test different aspects of the solutions in order to ensure the correct behavior of our IMEX-RK2 scheme.

Keywords: Conservation laws, WENO schemes, IMEX schemes, Numerical schemes, Chromatography.

MSC 2010: 35L40, 35L45, 35L65, 35L67, 65M06, 65M22, 65F10, 65H17

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Stability and bifurcation of a capillary fluid on an infinite cylinder

Rafael López[1],

We consider a fluid of an incompresible and homogeneous liquid partially wetting the exterior surface on an infinite solid cylinder Σ where the only force is the surface tension and the effect of gravity is negligible. The shape of the air-liquid interface M arises from minimizing the energy $E = |M| - c|W|$, where $|M|$ is the area of M, $|W|$ is the area of the wetted region by the fluid on Σ, and the constant $c \in (-1, 1)$ depends on the material of Σ. The minimization is under the constraint that the volume of the fluid is fixed and the contact curves are free to move on Σ. It follows from the Young-Laplace equation that the first variation of E is zero if and only if the mean curvature H of M is constant and the angle between the unit normal vectors to M and Σ is a constant $\gamma \in (0, \pi)$ along the curve of contact, where $\cos \gamma = c$. In such a case, we say that M is a capillary surface on Σ.

In this talk we assume that the fluid is invariant in the directions of the axis of Σ. In particular, we suppose that the free surface M of the fluid is a cylinder that meets Σ (different radii) along two meridians and with contact angle γ. Among the different shapes of the interface, we are interested on stable capillary surfaces because they are the configurations that can be physically realizable. The study of the stability of a circular cylinder has appeared in many physical settings ([1, 3, 7, 8]) and it has been analyzed in [4, 5, 9]. Motivated by the classical Rayleigh instability criterion, we give a stability result in terms of the wavelength of M, determining when M is or is not stable [6]. This study is equivalent to an eigenvalue problem for the Jacobi operator with boundary conditions of Neumann type.

When the fluid loses the stability, the eigenvalues cross zero and the Jacobi equation has non-trivial solutions. In such a case, it is possible the appearance of new equilibrium shapes which bifurcate from the initial cylindrical fluid [1, 4]. Under certain configurations (radii and contact angle), we prove that the cylinder M bifurcates in a family of new surfaces of constant mean curvature and intersecting Σ with the same contact angle γ. Moreover these surfaces are periodic in the direction of the axis of Σ. The result that we use is the 'bifurcation at a simple eigenvalue"due to Crandall-Rabinowitz [2]. Here the mean curvature H (or equivalently the radius r) of M is the variable in the bifurcation argument. The bifurcation appears when the second eigenvalue is 0 and, in such a case, we need to prove that the corresponding eigenspace is one-dimensional. A detailed description of the eigenvalues allows to find those configurations of the fluid where the Crandall-Rabinowitz scheme can apply.

Keywords: capillary surface, cylinder, bifurcation, stability, simple eigenvalues

MSC 2010: 58E12, 49K30, 53A10

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Analysis of a parabolic-elliptic problem with moving parabolic subdomain through a Lagrangian approach

Rafael Muñoz-Sola[1]

Let Ω be a bounded domain of $\mathbb{R}^n$ with Lipschitz boundary, $\hat{\Omega} \subset\subset \Omega$ a subdomain with smooth enough boundary, $T > 0$ and $\mathbf{X} : [0,T] \times \overline{\hat{\Omega}} \mapsto \mathbb{R}^n$ be a smooth mapping such that: $\mathbf{X}(t,\cdot)$ is injective for all $t \in [0,T]$, $det(D_p\mathbf{X})(t,p) > 0$ for all $(t,p) \in [0,T] \times \overline{\hat{\Omega}}$, $\mathbf{X}([0,T]) \times \overline{\hat{\Omega}}) \subset \Omega$ and $\mathbf{X}(0,p) = p$ for all $p \in \overline{\hat{\Omega}}$. We denote $\Omega_t := X(t,\cdot)(\hat{\Omega})$. For $n = 3$, $\mathbf{X}$ represents a deformation of a body evolving smoothly with time. Let $\mu > 0$ be a constant, $\hat{\sigma} \in L^\infty(\hat{\Omega})$ such that $\hat{\sigma} \geq \underline{\sigma} > 0$ and let $\sigma \in L^\infty((0,T) \times \Omega)$ defined by: $\sigma(t,x) = \hat{\sigma}(p)$ if $x = \mathbf{X}(t,p)$ with $p \in \hat{\Omega}$, and $\sigma(t,x) = 0$ if $x \notin \overline{\Omega_t}$. Let $A^0 \in H^1(\hat{\Omega})$ and $f \in H^1(0,T;L^2(\Omega_S))$ be given data, where the open set $\Omega_S \subset \Omega$ and $\overline{\Omega_S} \cap \overline{\Omega_t} = \emptyset$ for all $t \in [0,T]$. The goal of this talk is to study the regularity of the following parabolic-elliptic initial-boundary value problem: find A s. t.

$$\left\{ \begin{array}{ll} \sigma \frac{\partial A}{\partial t} - \frac{1}{\mu} \triangle A = f & \text{in } (0,T) \times \Omega, \\ A = 0 & \text{on } (0,T) \times \partial\Omega, \\ A(\cdot,0) = A_0 & \text{in } \hat{\Omega}. \end{array} \right. \tag{1}$$

This problem is closely related to the model considered in [1] and [2] for the electromagnetic field produced by a coil in a cylindrical metallic workpiece undergoing a given deformation, under suitable assumptions of symmetry of the data. The model consists in the parabolic-elliptic PDE (written in cylindrical coordinates)

$$\sigma \frac{\partial A}{\partial t} \vec{e}_\theta + \nabla \times \left[\frac{1}{\mu} \nabla \times (A \vec{e}_\theta) \right] = J_S \vec{e}_\theta \quad \text{in } (0,T) \times (0,R) \times (0,L), \tag{2}$$

where J_S is the current density in the coil and $\vec{A} := A(t,r,z)\,\vec{e}_\theta$ is the magnetic vector potential. In [1] some results of existence, uniqueness and regularity were obtained for (2) (suplemented with an initial condition and an homogeneous Dirichlet condition), but the analysis of the convergence of the fully discrete numerical approximation introduced in [2] needs further regularity. Roughly speaking, it requires the $H^2(0,T;L^2(\Omega))$ regularity of the solution. For both problems, the fact that the PDE is parabolic only in the time-dependent set Ω_t makes difficult to study this regularity by using the approach of [1]. This approach is based in the Eulerian coordinates x for problem (1) (and in the cylindrical coordinates associated to x for problem (2)).
In this talk, we develop an approach based on the Lagrangian coordinate p to study

the regularity of the solution of (1). We start from the weak formulation of (1), namely:

$$\begin{cases} \text{Find } \ A \in L^2(0;T;H_0^1(\Omega)), \text{with } \frac{\partial A}{\partial t} \in L^2(Q) \quad \text{ s.t.} \\ \int_{\Omega_t} \sigma \frac{\partial A}{\partial t} v dx + \mu \int_{\Omega} \nabla A \cdot \nabla v dx = \int_{\Omega_S} f v dx \quad \forall v \in H_0^1(\Omega) \quad \text{ a.e. } \ t \in (0,T) \\ A(0) = A_0 \quad \text{ in } \hat{\Omega}, \end{cases} \tag{3}$$

where $Q = \{(t,x) \in \mathbb{R}^{n+1}, t \in (0,T), x \in \Omega_t\}$. First, since $\mathbf{X}$ is defined only in $[0,T] \times \overline{\hat{\Omega}}$, we construct an extension $\tilde{\mathbf{X}} : [0,T] \times \overline{\Omega} \mapsto \overline{\Omega}$ of $\mathbf{X}$ such that $\tilde{\mathbf{X}}$ is smooth, $det(D_p\tilde{\mathbf{X}})(t,p) > 0$ for all $(t,p) \in [0,T] \times \overline{\Omega}$ and $\tilde{\mathbf{X}}(t,\cdot) : \overline{\Omega} \mapsto \overline{\Omega}$ is a homeomorphism keeping invariant both Ω_S and $\partial\Omega$ for all $t \in [0,T]$.
By making the change of variables $x = \tilde{\mathbf{X}}(t,p)$ in the whole $(0,T)\times\Omega$, we reduce (3) to the weak formulation of an parabolic-elliptic problem with variable coefficients for the function $\hat{A}(t,p) := A(t, \tilde{\mathbf{X}}(t,p))$, but now the parabolic subdomain is $\hat{\Omega}$, hence independent of time.
In a further step we introduce an Steklov-Poincaré (that is, Dirichlet to Neummann) operator associated to the elliptic problem which $\hat{A}(t)$ satisfies in $\Omega^e := \Omega\backslash\overline{\hat{\Omega}}$. This enables to reduce further the problem to a non-degenerate parabolic problem posed in $(0,T) \times \hat{\Omega}$ with a non-local boundary condition involving the Steklov-Poincaré operator. This parabolic problem is a special case of an abstract parabolic problem of the form

$$\begin{cases} \text{Find } \ u \in L^2(0;T;V) \cap H^1(0;T;H) \quad \text{ s.t.} \\ B(t)\frac{du}{dt} + E(t)u + C(t) = F(t) \\ u(0) = u_0, \end{cases} \tag{4}$$

where V and H are Hilbert spaces satisfying the usual assumptions (see, for instance, [3]), $B(t) \in \mathcal{L}(H)$, $E(t) \in \mathcal{L}(V;V')$, $C(t) \in \mathcal{L}(V;H)$, $F \in H^1(0,T;V')$ and $u_0 \in V$. By deriving a priori estimates, we obtain regularity results for (4) in terms of the smoothness of the operator coefficients, which generalize classical results ([3]).
Next, we apply these results to our concrete problem. In this case the operator $E(t)$ involves the Steklov-Poincaré operator and hence an elliptic problem with time-dependent coefficients.
In this way we obtain regularity results for the restriction of $\hat{A}$ to $(0,T)\times\hat{\Omega}$. Then, by analyzing the elliptic problem which $\hat{A}(t)$ satisfies in Ω^e, we obtain regularity results for the restriction of $\hat{A}$ to $(0,T) \times \hat{\Omega}^e$.
Finally, we use again the change of variables $x = \tilde{\mathbf{X}}(t,p)$ to obtain the regularity of A from that of $\hat{A}$.

Keywords: Parabolic-elliptic problem, moving parabolic subdomain, Lagrangian

MSC 2010: 35K20, 35K65

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A local ADER FV/FE projection method for Navier-Stokes equations with turbulence and species transport

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The scope of this talk is to present a second order in space and time finite volume/finite element projection method to solve the Navier-Stokes equations. Moreover, transport of species, energy conservation laws and a $k - \varepsilon$ standard model will also be considered (see [1]).

Starting with a 3D tetrahedral finite element mesh of the computational domain, the momentum equation is discretized by a finite volume method associated with a dual finite volume mesh. The resolution of Navier-Stokes equations coupled with a $k-\varepsilon$ turbulence model requires the use of a high order scheme. The ADER methodology for solving advection-diffusion-reaction equations (see [2]) is extended to 3D. The developed Local ADER method profits from the dual mesh and uses the Galerkin approach to reduce the stencil and the computational cost. The obtained scheme is second order in space and time.

Concerning the projection stage, the pressure correction is computed by a piecewise linear finite element method associated with the initial tetrahedral mesh. Passing the information from one stage to the other is carefully made in order to get a stable global scheme (see [3]).

Finally, the analysis of the order of convergence by means of academic problems and several classical test problems from fluid mechanics are presented.

Keywords: Navier-Stokes, RANS $k - \varepsilon$, Finite Volumes, ADER methodology, Finite Elements

MSC 2010: 35L00, 35Q00, 65M00, 76D00, 76F06, 76M01, 76M02, 76R01, 76R02

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Viscoelastic biodegradable materials: modelling, mathematical analysis and medical applications

Paula de Oliveira[1]

Viscoelastic properties of materials represent a compromise between viscous and elastic responses, under mechanical stress. Biodegradation is the erosion of materials by the action of biological processes that cause a progressive breakdown of the material. The degradation and the unique viscoelastic properties of polymers give them a central role in controlled drug delivery to provide sustained release of therapeutic agents while avoiding removal surgery.

The release of drug is governed by an instantaneous swelling, a nonlinear diffusion, a stress driven convection and a decrease of the polymer molecular weight. The interaction of these phenomena is represented by a system of partial integro-differential equations, coupled with initial and boundary conditions. The qualitative properties of the solution are studied and the stability of the system is analyzed.

Medical applications are addressed. In vivo evolution of the concentration of drug, released from a biodegradable viscoelastic implant, is analyzed. Numerical simulations illustrate how to tune polymeric material properties that give rise to predefined release profiles.

The material presented in this talk is a joint work with J. Ferreira and P. Silva.

Keywords: Drug release, viscoelastic polymers, biodegradable implant

MSC 2010: 35K55, 65N06

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Continuation of periodic orbits in domains heated by the side

Marta Net[1], **Juan Sánchez Umbría**[1]

The usefulness and advantages of computing periodic solutions of dissipative PDEs by means of Newton-Krylov continuation methods [1, 2, 3] will be illustrated in the presentation with the application of the method to the calculation of the periodic flows arising in a tall rectangular cavity laterally heated. This problem has long been studied because of its relevance in industrial applications, for instance, in the successful growth of single liquid crystals, the design of large-scale laser systems, or the optimal heating or cooling and isolation of buildings.

It was known that in this problem there are multiple stable periodic and quasiperiodic orbits coexisting in the same range of parameters, which origin was assumed in [4] from the comparison of the critical eigenfunction of the steady solutions at the bifurcating points and the spatial and temporal structure of the periodic orbits. Here it is shown that the orbits detected previously by time evolution (and other branches calculated only by continuation techniques) arise directly from the basic steady flow without intermediate turning points or symmetry-breaking bifurcations. The Neimark-Sacker points on the branches of periodic solutions have been determined with precision for a long range of Rayleigh numbers.

Keywords: Periodic orbits, Bifurcations and Stability, Thermal convection

MSC 2010: 37G15, 76Exx

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Quasiconvexity, Rank-One Convexity and the Non-Negativeness of Polynomials

Luís Bandeira[1], **Pablo Pedregal**[2]

We report our work about non-negativeness of polynomials and the main necessary and sufficient conditions for weak lower semicontinuity of integral functionals in vector calculus of variations. The celebrated theorem about sum of squares and non-negativeness of polynomials, due by David Hilbert, plays a special role, providing new tools to investigate rank-one convexity of functions defined on 2×2-matrices. For these results, we explore some consequences and examples.
We also explore the relationship between quasiconvexity and non-negativeness of certain polynomials, in particular, the case where the integrand of an integral functional is a fourth-degree homogeneous polynomial.

Keywords: Quasiconvexity, Rank-one Convexity, Polynomials, Sums of Squares

MSC 2010: 49J45, 49J10.

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On the minimization of the urban heat island effect in metropolitan areas

Lino J. Alvarez-Vázquez[1], **Francisco Fernández**[2], **Aurea Martínez**[1], **Miguel E. Vázquez-Méndez**[3]

In this work we combine optimization techniques, numerical simulation and optimal control theory of partial differential equations in order to mitigate the *urban heat island* (UHI) effect: a very usual environmental phenomenon where the metropolitan areas present a significantly warmer temperature than their surrounding areas, mainly due to the consequences of human activities. The temperature difference between urban areas and the surrounding suburban or rural areas can reach upto 5 degrees. These temperature differences are larger at night than during the day, and is strongly marked when winds are very weak. At the present time, UHI is considered as one of the major environmental problems in the 21st century as an undesired result of urbanization and industrialization of human civilization [1]. Mitigation of the UHI effect can be accomplished through the use of green roofs or of lighter-coloured surfaces in urban areas, or - as will be addressed in this study - through the setting of new green zones inside the city. So, we introduce a well-posed mathematical formulation of the environmental problem (related to the optimal location of green zones in metropolitan areas), we propose a numerical algorithm for its resolution, and finally we present several numerical results.

Keywords: Partial differential equations, Optimal control, Urban heat islands

MSC 2010: 35B37, 49J20

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Second-order structured deformations: relaxation, integral representation and applications

Ana Cristina Barroso[1], **José Matias**[2] **Marco Morandotti**[3] **David R. Owen**[4]

Second-order structured deformations of continua provide an extension of the multiscale geometry of first-order structured deformations by taking into account the effects of submacroscopic bending and curving. In this talk an integral representation for a relaxed energy functional in the setting of second-order structured deformations is presented. Our result covers inhomogeneous initial energy densities (i.e., with explicit dependence on the position in the given body). Explicit formulas for bulk relaxed energies in a particular example, as well as some applications, are also provided.

Keywords: structured deformations, relaxation, energy minimisation

MSC 2010: 49J45, 74G65, 74M25

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Optimal Design of Fractured Media with Prescribed Macroscopic Strain

José Matias[1], **Marco Morandotti**[2] **Elvira Zappalle**[3]

In this work we consider an optimal design problem for two-component fractured media for which a macroscopic strain is prescribed. Within the framework of structured deformations, we derive an integral representation for the relaxed energy functional. We start from an energy functional accounting for bulk and surface contributions coming from both constituents of the material; the relaxed energy densities, obtained via a blow-up method, are determined by a delicate interplay between the optimization of sharp interfaces and the diffusion of microcracks. This model has the far-reaching perspective to incorporate elements of plasticity in optimal design of composite media.

Keywords: Structured deformations, optimal design, relaxation

MSC 2010: 49J45 , 74A60

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Modeling the physiopathology of the vascular system

Jorge Tiago[1], **Telma Guerra**[2], **Telma Silva**[3], **Adélia Sequeira**[4]

Vascular diseases, such as brain aneurysms and atherosclerosis, are the main cause of death in the western countries. Such pathologies are not fully understood and lack precise diagnosis procedures. The mathematical modeling of blood flow in the cardiovascular system, both in normal and pathological conditions, may be the way to provide a computational tool to be used for diagnosis, prognosis or training purposes. In this sense, accurate numerical simulations must be achieved, in order to be considered reliable. However, this can be a challenge since important data, needed to close the mathematical model, is usually missing. To overcome such difficulty, variational data assimilation techniques can be used. Besides, in the case of complex pathologies, such as atherosclerosis, a cascade of biochemical and biomechanical factors must be modeled. Therefore, such models results in coupled systems of partial differential equations, which are non trivial from the analysis point of view. In this talk, we will discuss some mathematical and numerical aspects related to these issues.

Keywords: Blood flow, atherosclerosis, data assimilation, numerical simulations

MSC 2010: 92C, 35Q92, 49J20

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Differential equations subject to uncertainty: some connections between different approaches

Rosana Rodríguez-López[1]

One of the approaches to include uncertainty in mathematical models is fuzzy mathematics. Fuzzy differential equations have become an intensive field of research, motivating the development of several concepts of derivatives for functions with fuzzy values. This way, the concept of Hukuhara differentiability has been completed with other generalized concepts such as strongly generalized derivative or generalized Hukuhara differentiability. Besides, other techniques have been proposed in order to deal with this type of equations, we mention, for instance, Zadeh's Extension Principle or the solvability through differential inclusions.

It is well known that equivalent real differential equations might be no longer equivalent in the fuzzy context. Indeed, using the concept of a fuzzy differential to obtain a solution, the fuzzy solutions to related linear problems that are identical in the real case may exhibit very different behavior. Being Zadeh's Extension Principle a useful approach to avoid these drawbacks but presenting also some difficulties concerning the computational treatment, we consider here the approach of solutions based on strongly generalized differentiability [1, 2, 3], and the method of differential inclusions [5], which does not require the consideration of a concept of fuzzy derivative.

In particular, we establish some connections between the expression of the solution to linear fuzzy differential equations via differential inclusions and the corresponding strongly generalized solutions. This study is based on the explicit expression of the solutions to the Cauchy problem for linear fuzzy differential equations provided in [6]. Some related works on initial value problems are [4, 8], while some results for certain types of boundary value problems following different approaches can be found, for instance, in [7, 9].

Keywords: Fuzzy differential equations, Strongly generalized differentiability, Differential inclusions' approach

MSC 2010: 34A07, 34A30, 34A60, 26E50

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First results on the modelling of heavy metals phytoremediation

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This work deals with the numerical modelling of the different processes related to the phytoremediation methods for remediation of heavy metal-contaminated environments. Phytoremediation is a cost-effective plant-based approach of remediation that takes advantage of the ability of plants to concentrate elements and compounds from the environment and to metabolize them in their tissues (toxic heavy metals and organic pollutants are the major targets for phytoremediation).

Within the framework of water pollution, biosorption (which uses the ability of biological materials to remove and accumulate heavy metals from aqueous solutions) has received considerable attention in recent years because of its advantages compared to traditional methods. Biosorption uses cheaper materials (such as naturally abundant algae and microalgae) as biosorbents. Algae possess the ability to take up toxic heavy metals from the environment, resulting in higher concentrations than those in the surrounding water.

In order to analyse this environmental problem, we propose a bidimensional mathematical model coupling the system for shallow water hydrodynamics with the system of coupled equations modelling the concentrations of heavy metals, algae and nutrients in large waterbodies. In this first mathematical approach to the problem from the viewpoint of environmental control, we present a numerical algorithm for solving the system, and several preliminary computational examples for a simple realistic case.

Keywords: Partial differential equations, Numerical modelling, Heavy metals

MSC 2010: 35B37, 49J20

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Two fractional differential equations in mechanics

Cao Labora, Daniel[1]

The main goal of the talk is to make an introduction to fractional calculus and to show its usefulness when dealing with two particular physical problems.

Fractional calculus studies integrals and derivatives of non-integer orders. Some reasonable ideas of how this generalization could be made are presented. We build the Riemann-Liouville fractional integral and an analogous expression for the associated fractional derivative is found too. The ideas of this first part can be found in [1].

The previous concepts allow to formulate two fractional differential equations (Abel equation and Bagley-Torvik equation) that are deduced from two physical problems. The first problem cares about finding the "tautochrone curve" and we will follow the basic lines exposed in [2]. The second one deals with the "motion of an immersed plate" and we will use [3].

Keywords: Fractional calculus, Tautochrone curve, Motion of an immersed plate

MSC 2010: 26A33

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Modelling air pollution due to traffic flow in urban networks

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Traffic flow is known as the main pollution source in urban zones. In big cities there exist several thousands of vehicles (even millions of them in megacities), so estimating the pollution emission rate due to traffic flow is a hard task.

To address this environmental issue, we propose a methodology consisting of combining the 1D Lighthill-Whitham-Richards (LWR) model with a classical 2D advection-diffusion-reaction pollution model. The pollution model uses a source term that takes into account the traffic flow contamination via a Radon measure supported on a road network in a 2D urban domain.

In this work we establish the existence of solution for the combining model, and detail a complete algorithm to solve it: using the supply-demand method for the LWR model with a characteristic Lagrange finite element method for the pollution model. Finally, some numerical experiments on a real urban domain: the Guadalajara metropolitan area (Mexico) are presented, where the final aims are addressed to the control of the air pollution.

Keywords: Partial differential equations, Numerical simulation, Traffic pollution

MSC 2010: 35B37, 49J20

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Simulación numérica en la U.P.T. de As Pontes

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Numerosos problemas relacionados con los fluidos tienen lugar en un central térmica de carbón pulverizado como es la que la empresa Endesa tiene en As Pontes. En esta comunicación se abordará el análisis de flujo bifásico, compresible, turbulento y reactivo que tiene lugar en el interior de la caldera. Ello se ha abordado de dos formas diferentes: en primer lugar, definiendo los modelos matemáticos que describen los fenómenos físico/químicos de interés y, posteriormente, implementando los métodos numéricos que los resuelve y en segundo lugar, utilizando una herramienta de mecánica de fluidos comercial.

Así, empezaremos presentando el modelo matemático que se ha desarrollado para la combustión de carbón pulverizado (ver [1]), el cual incluye la evaporación de la humedad, la devolatilización y la gasificación del *char*, con la posibilidad de que ocurran de forma simultánea. Ese modelo se ha implementado en un código de elementos finitos, en el que se utilizan métodos numéricos análogos a los semilagrangianos y que serán presentados en otra ponencia de la sesión, y validado en [2], utilizando para ello los datos de una llama generada en un chorro de carbón pulverizado, y obteniendo resultados como el que se muestra en la Figura 1.

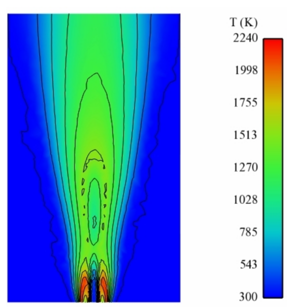

Figura 1: Temperatura de la mezcla gaseosa [K]

Por otra parte, utilizando un software comercial de Mecánica de Fluidos Computacional (CFD), se han simulado numéricamente algunos de los procesos que tienen lugar en una Central Térmica de carbón pulverizado como, por ejemplo, la organización de la combustión en el interior de la caldera y la distribución de gas y partículas de carbón en las cajas de viento (ver [3]) o en un quemador.

Keywords: pulverized coal combustion, mathematical model, CFD

MSC 2010: 80A25, 35Q35

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A numerical method for the space distributed order Riesz fractional diffusion equation

Magda Rebelo[1], **Luísa Morgado**[2]

In the recent decades a considerable and increasing attention has been devoted to fractional differential equations mainly because it has been observed that models including noninteger orders in their derivatives could describe accurately certain processes than those that restrict the orders of the derivatives to integer values.

Application problems of fractional differential equations are nowadays recognized in several areas of science and engineering, as Physics, Finance, Medicine, Biology and Biochemistry, just to name a few (see book [1]).

The Riesz fractional diffusion equation (RFDE) has been found in a broad variety of engineering, biological and physics processes. For example, for the modeling of the propagation of the electrical potential in heterogeneous cardiac tissue ([2] and [4]) and for modeling the growth and dispersion of population species ([3]).

In this work we analyse the numerical approximation of a generalization of RFDE, which may be achieved by considering the so-called distributed order equation. The Riesz fractional diffusion equation with distributed order may be written as:

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

where $c(\alpha)$ acts as a weight for the order of differentiation.

We present a first order (time and space) accurate implicit scheme for the numerical approximation of the distributed order RFDE with appropriate boundary and initial conditions. The unconditional stability and the convergence order of the numerical scheme are analysed and illustrated through some numerical examples.

Keywords: Fractional differential equation, Riesz derivative, diffusion equation, implicit finite difference method, stability

MSC 2010: 35R11, 65M06, 65M12

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Numerical solution of some Fokker–Planck kinetic equations

Óscar López Pouso[1]

The talk will be focused on the numerical solution of the Fokker–Planck equations

$$\mu \frac{\partial \psi}{\partial z} + \alpha \psi = \sigma \frac{\partial}{\partial \mu} \left[\left(1 - \mu^2\right) \frac{\partial \psi}{\partial \mu} \right] + W \tag{1}$$

and

$$\mu \frac{\partial \psi}{\partial z} + \alpha \psi = \sigma \left\{ \frac{\partial}{\partial \mu} \left[\left(1 - \mu^2\right) \frac{\partial \psi}{\partial \mu} \right] + \frac{1}{1-\mu^2} \frac{\partial^2 \psi}{\partial \theta^2} \right\} + W \tag{2}$$

accompanied by appropriate closing conditions. See [1] and references therein.

In Equations (1) and (2), $\psi = \psi(z, \mu, \theta)$ is the angular flux density of charged particles, and $\alpha \geq 0$, $\sigma > 0$, and W are given functions. Also, $(z, \mu, \theta) \in [Z_{\text{ini}}, Z_{\text{fin}}] \times [-1, 1] \times [0, 2\pi)$.

The solution to the Fokker–Planck equation is, under some circumstances, close to the solution to the Boltzmann equation, which may be much more difficult to solve.

Keywords: Fokker–Planck equation, finite differences, Crank–Nicolson scheme, two–way diffusion equations, continuous scattering operator.

MSC 2010: 35Q84, 65-05, 65Z05, 78M20, 78A35, 35K65.

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