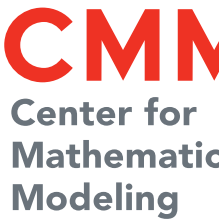

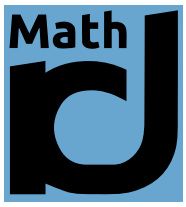

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Book of abstracts

Organizers: C.Bertoglio, C.Conca, G.Panasenko

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Spatial patterns and frequency distributions of regional deformation in the healthy human lung

Carlos Andrade, Pontificia Universidad Católica de Chile, Santiago, Chile

Since parenchymal deformation is crucial in respiratory physiology, the medical community has had a particular interest in the understanding of regional deformation in the lungs for a long time. The latest developments in image registration have made it possible to study regional deformation non-invasively, showing that volumetric deformation in healthy lungs follows complex spatial patterns not necessarily shared by all subjects, and that deformation can be highly anisotropic. In this work, we systematically study the regional deformation in the lungs of eleven healthy human subjects by means of in-vivo image-based biomechanical analysis. Regional deformation is quantified in terms of 3D maps of the invariants of the right stretch tensor, which are related to regional changes in length, surface and volume. Based on the histograms of individual lungs, we show that log-normal distributions adequately represent the frequency distribution of deformation invariants in the lung, which naturally motivates the normalization of the invariant fields in terms of the log-normal score. For a direct inter-subject comparison, normalized maps of deformation invariants are presented, since they exhibit spatial patterns of deformation in a range that is common to all subjects. Results showed that lungs in supine position display a marked gradient along the gravitational direction not only for volumetric but also for length and surface regional deformation, highlighting the role of gravity in the regional deformation of normal lungs under spontaneous ventilation.

Rupture risk estimation in thoracic aortic aneurysms

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Ascending thoracic aortic aneurysms (ATAA), described at tissue level by a biomechanical weakening of the aortic wall, are a life-threatening pathology provoking a permanent dilation with a high associated risk of aortic rupture or dissection and death of the patient. ATAAs affects approximately 10 out of 100 000 persons per year and are treated by replacing them with synthetic grafts when the aortic diameter exceeds 5.5 cm. However the rupture or the dissection of ATAAs remains rather unpredictable on a patient-specific basis. Even if the yearly risk of dissection or rupture rises from 3% to 7% with aneurysms >6 cm, rupture of ATAAs has been documented to occur at diameters less than 4.5 cm for more than 60% of patients. Other factors than the aneurysm diameter may also affect importantly the predisposition to rupture, such as age, hypertension, aortic valve phenotype or the presence of genetic disorders. In order to have a better insight in rupture risk prediction, our group developed a bulge inflation bench to test ATAAs samples collected on patients during surgical interventions. Stereo-digital image correlation (SDIC) was used to obtain the strain field of the inflated ATAA, allowing simultaneous evaluation of material parameters for constitutive modeling purposes and localized stress in the area that eventually ruptured. This proved to be a powerful experimental tool to characterize the mechanical properties of vascular tissues. Using this test, we derived the fracture properties on a cohort of 31 patients undergoing elective surgical repair and showed that these failure criteria based on ultimate strain correlate significantly with aortic distensibility that was measured pre-operatively with a dynamic CTscan. Finally, based on these results, we defined a new rupture risk assessing the brittleness of the tissue and we are now developing computational models based on growth and remodeling to predict the evolution of this rupture risk on a patient-specific basis.

Junction of models of different dimension for flows in tube structures: interface conditions involving pressure

Cristobal Bertoglio, Carlos Conca, CMM, UMI CNRS 2807, University of Chile, Santiago;
Grigory Panasenko, Institute Camille Jordan UMR CNRS 5208 and SFR MODMAD FED 4169, Univ. Lyon, UJM, F-42023, Saint-Etienne, France and CMM, UMI CNRS 2807, University of Chile, Santiago, Chile and
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Method of asymptotic partial decomposition of a domain (MAPDD) proposed and justified earlier for thin domains (rod structures, tube structures consisting of a set of thin cylinders) generates some special interface conditions between three-dimensional and one-dimensional parts (see[1-3]). In the case of fluid mechanics these conditions prescribe a pre-computed Poiseuille-type shape of a solution at the interface. Although it gives a high order precision for the non-steady three dimensional Navier-Stokes equations in tube structures without boundary layer in time, it is not applicable in the case of presence of the boundary layer in time. In the present talk we formulate and justify a precise junction condition for this general case. Moreover, for the reason of numerical implementation a Dirichlet-type interface condition (prescribed shape) for the velocity may be undesirable. So several alternative interface conditions involving pressure are proposed and justified: the closeness of solutions of these hybrid dimension problems to the solution of the complete three-dimensional setting is proved.

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2. Panasenko G., Partial asymptotic decomposition of domain: Navier-Stokes equation in tube structure , C.R. Acad. Sci. Paris, v. 326, Série IIb, 1998, pp. 893-898.
3. Panasenko G., Pileckas K., Asymptotic analysis of the non-steady Navier-Stokes equations in a tube structure.I. The case without boundary layer-in-time. Nonlinear Analysis, Series A, Theory, Methods and Applications, 122, 2015, 125-168, http://dx.doi.org/10.1016/j.na.2015.03.008

Models of thin composite piezoelectric plates

Eric Canon, Institute Camille Jordan UMR CNRS 5208 and SFR MODMAD FED 4169, Univ. Lyon, UJM, F-42023, Saint-Etienne, France, Michel Lenczner, FEMTO-ST, University Franche-Comté, France

We present models of thin composite elastic plates with periodically distributed piezoelectric inclusions and distributed electronic circuits. There are two small parameters, the thickness of the plate and the characteristic size of the inclusions, that we let tend to zero in order to derive an effective two-dimensional homogeneous model. The equations of elasticity and piezoelectricity in there linear and static versions are considered. We use a "mix" of the plate theory and the two-scale convergence as a tool.

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Numerical scheme for the equation on the graph for a flow in a tube structure

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An asymptotic analysis of the time dependent three dimensional Navier-Stokes equation in a thin tube structure [1,2] leads to two types of equations for the pressure on the graph of the structure: one of them is a well-known Reynolds equation on the graph with Kirchhoff junction conditions at the nodes (it appears at the slow time scale) ; another equation is a new one proposed by G.Panasenko and K.Pileckas in [2,3]. It corresponds to the fast time scale and couples a one-dimensional, nonlocal in time problem on the graph with a heat equation in the cross-section of the tubes. In the present talk, a numerical finite element scheme is proposed for this problem and its convergence is proved.

1. Panasenko G., Pileckas K., Asymptotic analysis of the non-steady Navier-Stokes equations in a tube structure.I. The case without boundary layer-in-time. Nonlinear Analysis, Series A, Theory, Methods and Applications, 122, 2015, 125-168, http://dx.doi.org/10.1016/j.na.2015.03.008

2. Panasenko G., Pileckas K., Asymptotic analysis of the non-steady Navier-Stokes equations in a tube structure. II. General case. Nonlinear Analysis, Series A, Theory, Methods and Applications, 125, 2015, 582-607, http://dx.doi.org/10.1016/j.na.2015.05.018

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An evolutionary perspective on cancer, with applications to anticancer drug resistance modeling and perspectives in therapeutic control

Jean Clairambault, Jacques-Louis Lions Laboratory, INRIA Mamba Team & UPMC, Paris, France

An evolutionary viewpoint on cancer will be presented, seen at the 2 time scales of (large-time) evolution in the genomes and of (short-time) evolution in the epigenetic landscape of a constituted genome. These widely metaphoric views, based on works by Lineweaver, Davies and Vincent (cancer as anatomically localized backward evolution in multicellular organisms) and by Sui Huang and collaborators (revisited Waddington epigenetic landscape), respectively, may serve as guidelines to propose a global conception of cancer, including towards possible innovating therapeutic strategies.

The question of drug-induced drug resistance in cancer will be considered in this framework, and a modeling setting, relying on phenotype-structured reaction-diffusion-advection equations, will be presented and interpreted biologically, speculating on the evolutionary mechanisms represented by the terms in the equations.

The built-in targets for theoretical therapeutic control present in our models are not supposed to represent well-defined molecular effects of the drugs in use, but rather functional effects, i.e., related to cell death (cytotoxic drugs), or to proliferation in the sense of slowing down the cell division cycle without killing cells (cytostatic drugs). We propose that cell life-threatening drugs (cytotoxics) induce by far more resistance in the highly plastic cancer cell populations than drugs that only limit their growth (cytostatics), and that a rational combination of the two classes of drugs may be optimized to propose therapeutic control strategies to avoid the emergence of drug resistance in tumors.

The models used are nonlocal Lotka-Volterra-like integro-differential equations, controlled by continuous inputs (representing drug delivery flows) to be optimised. Some theorems will be mentioned, and simulations will illustrate the biological and medical situations under description. Possible therapeutic consequences will be discussed.

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Determining the distribution of ion channels from experimental data using the Mellin transform

Carlos Conca, Department of Engineering Mathematics Center for Mathematical Modelling, UMI 2807 CNRS-UChile & Center for Biotechnology and Bioengineering University of Chile

We study an integral inverse problem arising in the biology of the olfactory system. The transduction of an odor into an electrical signal is accomplished by a depolarising influx of ions through cyclic-nucleotide-gated (CNG for short) channels on the cilium membrane. The inverse problem studied in this paper consists in finding the spatial distribution of the CNG channels from the measured transduce electrical signals. The Mellin transform allows us to write an explicit formula for its solution. Proving observability and continuity inequalities is then a question of estimating the Mellin transform of the kernel of this integral equation on vertical lines. New estimates using arguments in the spirit of the stationary phase method are obtained and a numerical scheme is proposed to reconstruct the density of CNG channels from laboratory data for an approximated model. For the original model an identifiability and a non observability (in some weighted L^2 spaces) results are proven.

Spatial modelling of tumour drug resistance: the case of GIST liver metastases

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Work in collaboration with Guillaume Lefebvre, Francois Cornelis, Thierry Colin, Clair Poignard and Olivier Saut.

This work is devoted to modelling gastrointestinal stromal tumour metastases to the liver, their growth and resistance to therapies. More precisely, resistance to two standard treatments based on tyrosine kinase inhibitors (imatinib and sunitinib) is observed clinically. Using observations from medical images (CT scans), we build a spatial model consisting in a set of non-linear partial differential equations. After calibration of its parameters with clinical data, this model reproduces qualitatively and quantitatively the spatial tumour evolution of one specific patient. Important features of the growth such as the appearance of spatial heterogeneities and the therapeutical failures may be explained by our model. We then investigate numerically the possibility of optimizing the treatment in terms of progression-free survival time and minimum tumour size reachable by varying the dose of the first treatment. We find that according to our model, the progression-free survival time reaches a plateau with respect to this dose. We also demonstrate numerically that the spatial structure of the tumour may provide much more insights on the cancer cell activities than the standard RECIST criteria, which only consists in the measurement of the tumour diameter. Finally, we discuss on the non-predictivity of the model using only CT scans, in the sense that the early behaviour of the lesion is not sufficient to predict the response to the treatment.

Keywords: tumour growth modelling; partial differential equations; cancer; drug resistance; tumour heterogeneity.

In silico radiobiological models and applications in radiotherapy

Ignacio Espinoza, Institute of Physics, Pontificia Universidad Católica de Chile, Santiago, Chile

In radiotherapy, it is important to predict the response of tumours to irradiation prior to the treatment. This is especially important for hypoxic tumours, which are known to be highly radioresistant. Mathematical modelling based on the dose distribution and biological input parameters may help to improve this prediction and to optimize the treatment plan. In this talk a radiobiological model is presented, which simulates the growth and the response to radiotherapy of macroscopic (clinical) tumours considering patient-specific information. The model considers the following biological processes: tumour growth, accelerated proliferation, hypoxia-induced angiogenesis, oxygen-dependent cell killing, resorption of dead cells and shrinkage. Anatomical and functional medical images may be used for the initial characterisation of the tumour. To simulate the response of hypoxic tumours properly, special emphasis is put on the description of the intratumoural oxygenation. For this, a second complementary model was developed to simulate the microscopic oxygen distribution, considering as input the vascular fraction per voxel, which is in principle measurable non-invasively in patients, and assuming certain simulated vascular architectures. The oxygen distribution is obtained by solving a reaction-consumption equation numerically. Including the fractionation regime and the planned dose distribution of the radiation treatment, the spatial-temporal behaviour of the tumour is simulated. The tumour control probability can be calculated as well. In this talk, some applications (e.g. dose-painting-by-numbers and alternative fractionation schemes analysis) and improvements (simulation of realistic 3D tumour vascular architectures) of the model are also presented.

The small amplitude homogenization method for optimal design

Sergio Gutiérrez, Structural and Geotechnical Engineering, Pontificia Universidad Católica de Chile, Santiago, Chile

Some Design Problems in Engineering can be formulated as optimization problems and they can be approximately solved using, for example, Finite Elements software. The problem that has received by far more attention in the academic literature is the minimization of the global deformation of a structure made-up of two elastic materials in given volumes, the so-called compliance minimization problem. In this talk we present the formulation of the Small Amplitude Homogenization method for optimal design, which can treat very general objective functions, at the price of assuming that the two materials being used are not very different, for example in terms of their stiffness, however, ratios 1:2 are still acceptable for specific problems.

The method is multiscale, since the mesoscale appearing due to the approximate relaxation of the optimization problem, can be solved separately from the macroscale optimization of the material distribution, even more, the mesoscale turns out to be independent of the macroscale (but not conversely), which greatly enhances the computational efficiency of the implemented codes. We present numerical results for two applications in the context of linear elasticity: compliance minimization under a constraint on stress concentration and nondestructive testing. For the latter we can also report on results of laboratory experiments.

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Fracture by void growth and coalescence

Duvan Henao, Facultad de Matemáticas, Pontificia Universidad Católica de Chile

We present a free-discontinuity model, based on nonlinear elasticity, for the nucleation, growth and coalescence of voids in materials with high resistance to volume changes. We prove rigorously the variational convergence of a phase-field regularization and present some numerical results. This is joint work with Carlos Mora-Corral (UAM, Madrid) and Xianmin Xu (CAS, Beijing).

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Boundary integral formulation and semi-implicit scheme for modeling packed cells under electrical stimulation

Fernando Henríquez, Seminar for Applied Mathematics, ETH Zurich, Zurich, Switzerland
Carlos Jerez Hanckes, School of Engineering, Pontificia Universidad Católica de Chile, Santiago, Chile

We model the electrical behavior of large numbers of biological cells under external stimuli by extending and computationally improving the semi-implicit multiple traces formulation presented in (Henríiquez *et al*., Numerische Mathematik, 2016). As customary, the electric current across each cell membrane is characterized by a capacitive term, due to potential jumps, plus an ionic one, modeled by systems of ordinary differential equations. However, when considering electrical interactions among multiple cells, traditional methods quickly become impractical due to the non-local entwinement potential jumps and currents. Our method leverages on smoothness of cellular shapes as extra regularity of solutions allows for spatial spectral discretization bases instead of conventional boundary elements, thereby largely reducing the degrees of freedom. Time-space coupling is achieved via a semi-implicit time-stepping scheme shown to be stable and convergent. We present numerical results in two dimensions validating our claims as well as matching observed biological behavior.

F. Henríquez, C. Jerez-Hanckes, F. Altermatt, *Boundary Integral Formulation and Semi-Implicit Scheme Coupling for Modeling Cells under Electrical Stimulation*, Numerische Mathematik (2016), DOI: 10.1007/s00211-016-0835-9.

Seventh International Conference on Multiscale Modelling and Methods: Upscaling in Engineering and Medicine, Santiago, Chile, January 2017

Model quantification of axon responses to kilohertz-frequency spinal cord stimulation for the treatment of chronic pain

Leonel Medina, Duke University, USA and Warren Grill, Duke University, USA

Background: Kilohertz-frequency spinal cord stimulation (KHF-SCS) was recently proposed as a paresthesia-free treatment for persons with chronic pain that is potentially more effective than conventional (~ 50 Hz) SCS. In SCS, the applied electrical stimulation is intended to activate the dorsal column (DC) axons. However, it is unclear how DC axons respond to kilohertz frequency signals. We developed a model of a DC fiber to quantify the responses of DC axons to the KHF-SCS signal.
Methods: We implemented a microscopic biophysical model of electrical excitation of a DC axon that we coupled to a realistic macroscopic electromagnetic model of SCS. The DC axon was modeled using published morphological data, and Hodgkin-Huxley ion channel dynamics. We used magnetic resonance images to implement a patient-specific volume conductor model of SCS. The computed potentials were then applied to quantify thresholds for activation and conduction block for different axon diameters at different locations in the DCs. We quantified the degree of synchronization of the firing activity to the stimulation signal using the vector strength, and the similarity between the activities of pairs of fibers using the normalized spike time distance.
Results: Activation thresholds using the KHF-SCS signal increased sharply as the axons were placed deeper in the DCs. For the most superficial axons (< 500 mm from the surface of the spinal cord), the activation thresholds for one patient averaged 57.2 ± 10.1 mA, 19.1 ± 6.1 mA and 8.3 ± 3.2 mA for fiber diameters of 2, 6 and 10 mm, respectively. The vector strength over the 10 – 50 mA amplitude range averaged 0.16 ± 0.09 and 0.11 ± 0.08 for 6 and 10 mm diameter fibers, respectively, indicating a low degree of synchronization to the KHFSCS signal. For any given signal amplitude, the spike time distance decreased as the axons were placed at closer distances, but it was always greater than 0.5.
Conclusion: Our model results showed thresholds for activation and block of DC axons well above the amplitudes used clinically (1 – 5 mA). If the KHF-SCS signal activates large superficial axons, then the axons would fire asynchronously to the stimulation signal and to other axons.

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A reduced model to detect low contrast inclusions in poroelastic media

Joaquín Mura, Biomedical Imaging Center, School of Engineering, Pontificia Universidad Católica de Chile.

In this talk, it is introduced a numerical method to detect elastic inclusions slightly stiffer or softer than its saturated poroelastic media matrix. In this kind of problems, the detection of low contrast inclusions is, in general, a difficult task. In order to tackle this issue, the detection of inclusions is formulated as a shape optimization problem composed by (i) a reduced model obtained from Biot's equations and (ii) the explicit computation of gradients using small-amplitude homogenization method. This method allows us to quickly identify inclusions in an efficient manner. Numerical simulations show excellent results when the contrast is below to 30% with a noise level below 5%.

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Role of small size ionic and conduction heterogeneities in the onset and dynamics of cardiac arrhythmias.

Alexander V.Panfilov, Gent University, Gent, Belgium

Cardiac arrhythmias account for about 1 death in 10 in industrialized countries. Although cardiac arrhythmias has been studied for well over a century, their underlying mechanisms remain largely unknown. Over the years, several factors that favor arrhythmias initiation were established. Among them are ionic and dynamical heterogeneity, remodeling and fibrosis of cardiac tissue. The present talk presents the recent studies of our team on the role of these arrhythmogenic factors performed using anatomically accurate model of ventricles of the human heart developed in our group.
In particular, it will be addressed a possible role of small size ionic heterogeneities found the human heart on the onset and dynamics ventricular arrhythmias. We show that they can attract and anchor the rotors. Further I discuss a role of heterogeneous fibrosis on the onset of cardiac arrhythmias. Our results show that spatial heterogeneity of fibrosis increases the probability of arrhythmia induction. We also show that properties of arrhythmias in such conditions are mostly determined by the maximal local fibrosis level. Based on that we hypothesize that it may be explained by the attraction of the rotors to the fibrotic scar. We further study this process and demonstrate that rotors indeed can be attracted by fibrotic scars via the process of dynamical reorganization of the excitation pattern which we call dynamical anchoring. We illustrate this process using patient specific model of the heart.

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Asymptotic analysis of a micropolar thin film flow with rough boundary and Tresca fluid-solid interface law

Laetitia Paoli, Institute Camille Jordan UMR CNRS 5208 and SFR MODMAD FED 4169, Univ. Lyon, UJM, F-42023, Saint-Etienne, France

We consider a non-stationary micropolar fluid flow in a 2D domain with a rough boundary. We assume that the thickness and the roughness are both of order ε ($0< \varepsilon<<1$). We assume also that the fluid is subjected to mixed boundary conditions with a given time-dependent velocity on a part of the boundary and Tresca's friction law on the other part. We prove the existence and uniqueness of a solution of this problem for any value of ε and we establish some a priori estimates. Then we use the two-scale convergence technique to derive the limit problem when ε tends to zero. Moreover we show that the limit velocity and micro-rotation fields are uniquely determined via auxiliary well-posed problems and the limit pressure is given as the unique solution of a Reynolds equation.

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Multiscale hybrid-mixed methods

Diego Paredes, Institute of Mathematics, Pontificia Universidad Católica de Chile, Santiago, Chile
Work in collaboration with R. Araya, F. Valentin and C. Harder.

This work proposes a Multiscale Hybrid-Mixed (MHM) method. The MHM method is a consequence of a hybridization procedure, and emerges as a method that naturally incorporates multiple scales while provides solutions with high-order precision. The computation of local problems is embedded in the upscaling procedure, which are completely independent and thus may be naturally obtained using parallel computation facilities. In this talk, we present this approach for different models. We address some theoretical aspects of the method and propose an extensive numerical validation. We conclude that the MHM method is naturally shaped to be used in parallel computing environments and appears to be a highly competitive option to handle realistic multiscale boundary value problems with precision on coarse meshes.

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[2] C. Harder, D. Paredes, and F. Valentin. On a multiscale hybrid-mixed method for advective- reactive dominated problems with heterogenous coefficients. SIAM Multiscale Model. and Simul., Vol. 13, No. 2, pp. 491–518, 2015.

[3] D. Paredes, F. Valentin and H. M. Versieux On the robusteness of multiscale hybrid-mixed Methods. Math. Comp., Vol. 86 No. 304, pp. 525-548, 2016.

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Schwarz waveform relaxation method for river hydraulics and coastal oceanography

Antoine Rousseau, INRIA, Equipe LEMON, Membre associé de l'Institut Montpelliérain A. Grothendieck, 34095 Montpellier,France

We consider multi-physics computational models. The idea is to couple equations at different scales and regimes, sometimes different dimensions. In this approach, 3 main questions will be addressed: 1) what are the relevant (simplified) models, 2) what type of interface conditions should be used and 3) where should the interface be located. We will provide numerical examples in river hydraulics, together with first results in Green-Neghdi / Saint-Venant coupling in coastal oceanography.

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Domain decomposition methods in a geometrical multi-scale domain using finite volume schemes.

Marie-Claude Viallon, Institute Camille Jordan UMR CNRS 5208 and SFR MODMAD FED 4169, Univ. Lyon, UJM, F-42023, Saint-Etienne, France

Finite volume schemes to solve a parabolic linear partial differential equation in a geometrical multi-scale domain are studied. The model domain consists of a central node, which is assumed to be two-dimensional (2D), and several outgoing branches, which are assumed to be one-dimensional (1D). Several domain decomposition methods are defined and com pared. Many of these methods are adapted from classical methods (Neumann-Dirichlet, optimized Schwarz,...). An iterative coupling strategy is applied to solve the interface problem. The interaction between subdomains is implemented by the means of boundary conditions on the interfaces, we compare the use of Dirichlet, Neumann and Robin conditions.

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Characterization of multiscale material properties of bioceramic bone scaffolds

Juan F. Vivanco, Facultad de Ingeniería Universidad Adolfo Ibáñez, Viña del Mar, Chile

Bone scaffolds have been considered potentially viable structures in regenerative medicine to support, guide and stimulate tissue growth. There has been a considerable rise in the interest of using calcium phosphate based bioceramic materials, such as hydroxyapatite and tricalcium phosphate, to serve as scaffolds due to their inherent biocompatibility, osteoconductivy, osteointegrity, and chemical similarity to the mineral phase of bone. Sintering, a well-known manufacturing method to fabricate bioceramics, can be an important determinant of materials and mechanical scaffold's properties at different length scales. This in turn, influences the optimal osteogenic signal expression and subsequent differentiation of cells seeded on the scaffold in both in vivo and in vitro conditions. Furthermore, in order to extend the use of bioceramic bone scaffolds to load-bearing applications, a comprehensive understanding of the mechanical properties should be investigated prior to implantation. Thus, the objective of this research was to investigate the sintering temperature effects on multi-scale properties of a macro-porous bioceramic bone scaffold regarding with respect to material, bioactivity, architectural, and multi-scale mechanical properties.

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Nonlinear dynamics of infection spreading in tissues

Vitaly Volpert, Institute Camille Jordan, UMR CNRS 5208

The immune system is regulated by multiple processes at various levels of biological organization. In this presentation we will discuss the interaction of viral infection with the immune response. We will use multi-scale models and delay reaction-diffusion equations in order to study nonlinear dynamics of infection spreading in tissues.