Symposium on Inverse Problems in Science and Engineering

Alain Kassab (University of Central Florida) Alain.Kassab@ucf.edu

RBF-Trained POD for Inverse Parameter Estimation and Optimal Design

Abstract:

André Novotny (Laboratorio Nacional de Computacao Cientifica) novotny@lncc.br

A New Non-Iterative Reconstruction Method for a Class of Inverse Problems

Abstract:

Several classes of inverse reconstruction problems are written in the form of over-determined boundary value problems. The general idea consists in rewriting them as an optimization problem. In particular, we are interested in the reconstruction of the support of a set of hidden anomalies embedded into a geometrical domain from partial boundary measurements. Therefore, a shape functional measuring the misfit of the solution obtained from the model and the data taken from the measurements is minimized with respect to a set of ball-shaped anomalies by using the concept of topological derivatives.

It means that the shape functional is expanded asymptotically and then truncated up to the desired order term. The resulting expression is trivially minimized with respect to the parameters under consideration, leading to a non-iterative second order reconstruction algorithm. As a result, the reconstruction process becomes very robust with respect to noisy data and independent of any initial guess.

Carlos J.S. Alves (Instituto Superior Tecnico de Lisboa) cjsalves@gmail.com

The Reciprocity Functional and its Application to the Solution of Inverse Problems

Abstract:

The notion of the Reciprocity Functional can be used together with Green's formulas to regularize boundary data and establish some techniques that allow the reconstruction in some inverse problems. We will consider different cases where this can be applied efficiently. For instance, if the inverse problem can be reduced to linear problems, we can obtain some formulas that express the solution with the help of auxiliary problems. Also, instead of fitting the Cauchy boundary data, the reciprocity functional can be used as a minimizer for an optimization scheme. Numerical experiments will be shown in the lecture.

Carolina Palma Naveira Cotta (Univ. Federal do Rio de Janeiro) cpncotta@hotmail.com

Experimental-Theoretical Analysis of Biodiesel Synthesis in Micro-reactors with Inverse Problem Solution for Parameter Estimation

Abstract:

The present talk deals with the analysis of the continuous synthesis of biodiesel in micro-reactors, with an innovative design that integrates micro-heat exchangers in the same substrate, so as to recover waste heat from a secondary thermal process to increase the reaction temperature. The final objective is to optimize efficiency in the biodiesel production using multiple micro-reactors/micro-heat exchangers modules, aiming at the scheduling of the production, with the desirable improvement in the conversion rates. The experimental analysis was carried out in a device composed of multiple 3D printed metallic micro-reactors with integrated micro-heat exchangers in the same substrate, thus reducing the overall thermal resistance. Such a device achieved an ethyl ester yield of 99.6% within a residence time of 35 seconds. A diffusive-convective-reactive three-dimensional mathematical model that describes the physico-chemical behavior of the species involved in the biodiesel synthesis is reformulated using the Coupled Integral Equations Approach (CIEA), resulting in a non-linear coupled mathematical model of first-order ODE's which allows for simulations with reduced computational costs. The Markov Chain Monte Carlo method (MCMC) is used to estimate the kinetic constants using real experimental data. It was then observed that experimental results with low conversion rates were necessary for a proper estimation, which maximizes the presence of the intermediary species and increases the sensitivity of the problem to the parameters.

Daniel Watzenig (Graz University of Technology) daniel.watzenig@tugraz.at

Statistical Modeling and Bayesian Inference for Industrial Applications

Abstract:

Bayesian inference applied to inverse problems provides a comprehensive framework for quantified model fitting, robust design, and parameter estimation. Key components in this framework are a prior model, the likelihood function that follows from a decomposition of measurements into deterministic and random parts and numerical simulation of noise-free measurements, the modeling of the underlying physics.

Uncertainty in recovered parameters arises from measurement noise, measurement sensitivities, model inaccuracy, discretization error and a priori uncertainty; each of these sources may be accounted for and in some cases taken advantage of. Estimates or properties of the unknowns can be calculated as summary statistics over the posterior distribution using e.g. Markov chain Monte Carlo sampling.

Several modified Metropolis–Hastings algorithms are available to speed up this computationally expensive step. A key difference between deterministic approaches (such as regularization) and Bayesian methods is that whereas regularization gives point estimates, typically using a data-misfit criterion, Bayesian methods present averages over all solutions consistent with the data. This leads to a marked difference in robustness of properties calculated from solutions. These differences occur because the single most likely solution, found by a regularized minimization of misfit to the measured data, is typically unrepresentative of the bulk of feasible solutions in high-dimensional nonlinear problems, which is the norm in inverse problems.

This talk discusses how parameter uncertainty can be quantified and taken into account in the estimation and optimization of process parameters conditioned on measurement data by several examples. More precisely, I will present three different industrial applications (process tomography, medical imaging, lithium-ion battery monitoring) and discuss the applied algorithms to estimate certain parameters and material properties in the presence of measurement noise and sensor imperfections. Current limits of the technology, recent advances and the roadmap beyond the state-of-the-art will be discussed in detail.

Denis Maillet (LEMTA, Université de Lorraine) DENIS.Maillet@univ-lorraine.fr

Experimental Identification of Transfer Functions for Diffusive and/or Advective Heat or Mass Transfer for Linear Time Invariant Dynamical Systems and Further Inverse

Abstract:

Experimental identification of transient heat diffusion and/or forced convection in a possibly heterogeneous physical system, governed by linear Partial Differential Equations whose coefficients are time independent, is considered here. If this system is stimulated by a separable source starting at initial time, the temperature variation at any of its points is a convolution product between the intensity of the source and its pulse response (an 'impedance' here). Consequently a convolution relationship also exists between temperatures observed at two distinct points [1]. Estimating the transfer function (a 'transmittance' here) linking these temperatures leads to a deconvolution problem, that becomes ill-posed if they are subject to measurement noise. The model of this linear inverse problem can be given a column vector/matrix form using a lower triangular Toeplitz matrix. Many different regularization techniques can be used for its inversion. Emphasis is put here on the fundamental problem of parameterizing the unknown transmittance and the interest of taking larger time steps for the transmittance than for the two sampled temperatures is highlighted.

References:
[1] W. Al Hadad, D. Maillet, Y. Jannot
Modeling diffusive and advective unsteady heat transfer for linear dynamical systems
Int. J. Heat Mass Transf. 115 (2017) 304-313

Fabio Bozzoli (Universita di Parma) fabio.bozzoli@unipr.it

Experimental Investigation about the Effect of Displaced Enhancement Devices on Local Convective Heat Transfer in Pipes

Abstract:

The actual work presents the original application of an inverse analysis technique to experimental infrared temperature data with the aim of estimating the local convective heat flux for forced convection flow in pipe with butterfly-shaped inserts. These inserts belong to the category usually named as 'displaced enhancement devices'. They are positioned inside the flow passage with the aim of increasing the heat transfer rate by “displacing” the fluid from the heated or cooled surface of the duct and mixing it with the core flow. In the present analysis water was adopted as working fluid in order to focus on the turbulent flow regime in ducts. The insert produces a distortion in the velocity profile that causes an irregular distribution of the wall heat flux along the circumferential coordinate. Several studies were carried out on displaced enhancement devices, but they were generally analysed by considering only the overall heat transfer performance. However, in some industrial applications, the knowledge of local thermal performances is of primary importance. The present work aims to fill this gap by presenting and testing an experimental procedure for estimating the local convective heat flux in pipes equipped with this type of inserts.

George S. Dulikravich (Florida International University) dulikrav@fiu.edu

Parameter Identification in Differential Equations: A Hybrid Minimization Based Method

Abstract:

Ordinary and partial differential equations and systems of such equations are most often used to model physical phenomena and processes. The terms multiplying derivatives in these equations account for the physical properties of the media and strongly influence the spatial and time variation of the field variables governed by such equations. It is of utmost importance to provide correct values of the properties of the media. Since these media properties can be space and time dependent, their modeling is typically performed using analytic functions of the space and time where such functions involve a number of unknown parameters. Determining correct values of these parameters is known as parameter identification. Since this is a de facto inverse problem of quantifying the causes (parameters) of the measured (or specified) field and/or boundary conditions, the identification process is typically referred to as inverse parameter identification (IPI). There are many methods for performing IPI, but most of them are highly mathematical, not sufficiently robust and not general. This paper discusses and presents examples of a simple, robust, accurate and completely general methodology for IPI that is based on non-destructive measurements, a relatively small number of high-fidelity analyses, and use of metamodels.

Gilmar Guimarães (Univ. Federal de Uberlandia) gguima@mecanica.ufu.br, gguima@ufu.br

Transfer Function Based on Green's Function Method (TFBGF) Applied to the Thermal Parameter Estimation

Abstract:

This study presents an unusual experimental technique to obtain the conductivity and thermal diffusivity of solid materials. In parameter estimation techniques properties are found minimizing an objective function. This function is usually a square function error calculated from the experimental and theoretical values of temperatures. In this case, the difficulty is the presence of local minima in the objective function when the parameters are correlated. Here, the proposed technique estimates the properties separately, but using the same experimental data. Heating and measurements of temperature and heat flux occur on the same surface. The method uses transfer function identification to solve inverse heat conduction problems. The technique is based on Green’s function and on the equivalence between thermal and dynamic systems. The basic idea here is the observation that the delay between experimental and theoretical temperatures in different positions is only function of the thermal diffusivity. This fact is the basis of the procedure to obtain the thermal diffusivity. Different objective functions are proposed to estimate thermal conductivity and diffusivity.

Guillermo Eliçabe (Universidad Nacional de Mar del Plata/CONICET) gelicabe@gmail.com

Thermal Parameter Identification in Remote Heating

Abstract:

This presentation addresses the estimation of the thermal parameters of a polymer matrix embedded with plasmonic nanoparticles using reduced models. The proposed problem corresponds to a remote heating based on the Photothermal Effect (PE) of a polymer by means of a laser beam. A 1D reduced model has been used to solve the forward radiative transfer problem involved, to achieve the equivalent thermal source. Time-varying and space-varying temperature measurements are simulated for a 3D-real geometry with additive Gaussian noise considering partial and total illumination from the beam. The corresponding solution for the thermal conductivity k and the heat capacity Cp is calculated using the Levenberg-Marquardt algorithm for 1D and 2D reduced geometries by the inversion of thermocouple temperature measurements at the center of the irradiated specimen. As a result, the scopes of the geometrically reduced models are evaluated in terms of the determination of these thermal parameters.

Haroldo de Campos Velho (Instituto Nacional de Pesquisas Espaciais) haroldo@lac.inpe.br

Parameter Identification in Mathematical Forecasting Models Depending on Prediction Time Scale

Abstract:

The dynamic of atmospheric circulation combines several phenomena in multi-scales for space and time. In addition, several phenomena occur simultaneously. The modeling approach of this dynamic is done by describing different processes in distinct coupled modules. One of these modules is the representation of surface coverage, since the dynamics depends on the interaction between the atmosphere and the soil. However, these modules depend on a number of parameters that need to be adjusted. The parameter adjustment process is called model calibration. Several atmospheric models uses the IBIS (Integrated Biosphere Simulator), including the Atmospheric Global Circulation Model (AGCM) from the CPTEC (Center for the Numerical Weather Prediction and Climate Studies), a division of the INPE (National Institute for Space Research), Brazil.

The IBIS model is calibrated following a multi-objective strategy. The Pareto set, which embraces the non-dominated solutions in the search space, is determined by a version of multi-objective genetic algorithm (NSGA-II). The model sensitivity to the parameters is evaluated by the Morris’ method. Data for calibration were obtained from the Tapajo?s National Forest (FloNa Tapajo?s), Brazil, located near to the 67 km from Santare?m-Cuiaba? highway (2.51S, 54.58W). We have also introduced the Epidemic Operator in the NSGA-II for improving the multi-objective genetic algorithm performance.

Jari Kaipio (University of Auckland) jari@math.auckland.ac.nz

Stochastic Boundary Maps and Uncertainties in Inverse Problems

Abstract:

In the majority of inverse problems that are induced by partial differential equations and the related boundary value problems, the computations cannot be carried out in the actual (physical) domain, but rather, in a small subdomain covering the region of interest. In such cases, the computational domain is (partially) enclosed by nonphysical boundaries on which the conditions are not generally known. Furthermore, in many cases, the exact geometry of the domain might not be exactly known. In this talk, we address these topics in the context of electrical impedance tomography.

Jose Herskovits Norman (Univ. Federal do Rio de Janeiro) jose@optimize.ufrj.br

Feasible Point Algorithm for Nonlinear Constrained Optimization and Some Applications to Parameter Identification in Structural Mechanics

Abstract:

This talk is based on FAIPA, the Feasible Arc Interior Point Algorithm for nonlinear constrained optimization. Given an initial feasible point, FAIPA generates a feasible descent sequence converging to the solution of the optimization problem. At each iteration a ``feasible descent arc'' is computed by solving two or three linear systems with the same matrix. The new iterate is obtained through a line search along the feasible descent arc. This search looks for a new feasible point with a lower objective function. FAIPA is supported by strong theoretical results. We prove global convergence to a Karush Kuhn Tucker point and that the rate of convergence is two-steps super-linear. Several test problems and applications in different disciplines were solved very efficiently with FAIPA. This approach showed to be robust, without need of parameters tuning. We also describe some applications of FAIPA to mechanical parameters identification of composite materials and sandwich structures.

Liliane Barichello (Univ. Federal do Rio Grande do Sul) lbaric@mat.ufrgs.br

On the Use of Analytical Techniques for Parameter Identification in Radiation and Particle Transport Models

Abstract:

Optical tomography and nuclear safety are some of the examples that may be cited as relevant problems, in particle transport theory, where parameter identification plays a significant role. In the first case, assuming the radiative transfer equation as basic model for the forward problem, one may be interested in estimating, in general, the absorption coefficient of the biological tissue. On the other hand, in safety analysis, the reconstruction of the source term, in the particle transport equation, is the main goal. In this work we discuss the use of analytical tools either for deriving, for instance, the adjoint operator and the entries of a fundamental matrix in the minimization process of the objective function for source reconstruction problems or for deriving spatially explicit solutions required in the forward problem of the absorption coefficient estimate. Numerical simulations are presented and analyzed.

Nilson Costa Roberty (Univ. Federal do Rio de Janeiro) nilson@con.ufrj.br

Reconstruction of Coefficients and Source Parameters in Elliptic Systems

Abstract:

Most of the stationary engineering models can be represented as elliptic systems of partial differential equations. Those models are mathematically elaborated with continuous thermomechanics and the constitutive theories of materials. Frequently we have incomplete information about parameters in coefficients and sources. This missing information is compensated with overspecification of data at the boundary. We analyze this kind of boundary value problems in Lipschitz domains by splitting Cauchy data at the boundary to formulate many direct problems, which for correct parameters values must have the same solution. The algorithmic trial of solutions with incorrect parameter values will generate an internal discrepancy between those solutions.

The main techniques adopted for the mathematical analysis of those problems are boundary integral equations reformulation of direct problems and the Calderon projector associated with the Cauchy data. In contrast to the use of mathematical concepts such as Calderon projector for the test of consistence of overprescribed Cauchy data and demonstration of phenomena of relation between the incorrect trial of parameters values and internal discrepancy of solutions, the numerical implementation of new methodology involves only solution of direct problems. To estimate those coefficients and sources we propose an optimization methodology based on this internal discrepancy observed when wrong parameter values are inserted in the constitutive equations. Nonlinear Least Squares or stochastic optimization can be used to search correct parameters in the inverse problems. Numerical experiments are presented.

Philippe Le Masson (IRDL, Universite de Bretagne - Sud) philippe.le-masson@univ-ubs.fr

Simulation of Welding: Estimation of Heat Sources and Multiphysical Modelisation

Abstract:

This seminar will have as object to present the activities around the welding through two points. Indeed, the simulation of welding can be approached by two manners. The first one is directed on a multiphysical simulation of the phenomena. This one includes the electromagnetism, the fluid mechanics, the thermal, the metallurgical transformations and the mechanics. This type of modelling is very time consuming in terms of calculations and requires a thorough knowledge of the material parameters in particular at high-temperature. The second leans on an equivalent model where the objective is the mechanical distortions and the residual stresses. For that purpose, it is imperative to determine the evolution of the thermal gradients versus time in the edge of the fused zone. In this case, a model purely conductive is developed and a heat source is parameterized by inverse method. During this seminar, two works will be presented. The first one concerns the parameter estimation of the heat source for a purely conductive model. The second will attempt to present a multiphysical approach in the case of welding of sheet steels by laser. A particular point will be made on the validity of the modelisations from the experimental data (measurements) and the parameters of the model.

Raul Lima (Universidade de Sao Paulo) lima.raul@gmail.com

The Design of Electrical Impedance Tomographs Using an Observability Concept

Abstract:

Frequently, sensors and actuators placement is decided in engineering products through concepts of observability and controllability, derived from the Control Theory. The present work addresses the problem of sensors and actuators placement for Electrical Impedance Tomographs using singular values of observability and controllability matrices as performance indices for design decisions. Numerical examples are used to show the correspondence of singular values and image quality.

Regina Almeida (Laboratorio Nacional de Computacao Cientifica) rcca@lncc.br

Selection, Calibration and Validation of Models of Tumor Growth

Abstract:

Cancer development results from a complex interplay of different phenomena that span a wide range of time and length scales. Computational modeling may help to unfold the role of multiple evolving factors that exist and interact in the tumor microenvironment. Understanding these complex multiscale interactions is a crucial step towards developing effective drug therapies. To this end, the reliability of model predictions is a major issue. Without some rigorous approach to assess model reliability in the presence of uncertainties, computer models are of limited value in medical science, or science in general. In this lecture, we will present an adaptive model selection and validation framework, based on the OPAL (Occam Plausibility Algorithm) concept, that brings together model-specific experimental data for model calibration, determination of sensitivities of outputs to parameter variances, calculation of model plausibilities for model selection, and development of criteria for the design of model validation experiments, in order to greatly improve the credibility of multiscale models of tumor behavior. We demonstrate these processes by comparing a list of models for tumor growth, including reaction–diffusion models, phase-fields models, and models with and without mechanical deformation effects, for glioma growth measured in murine experiments. Examples are provided that exhibit quite acceptable predictions of tumor growth in laboratory animals while demonstrating successful implementations of OPAL.

Rubens Sampaio (Pontificia Universidade Catolica - Rio de Janeiro) rsampaio@puc-rio.br

Smooth Modes as a Tool for Operational Modal Analysis: New Developments

Abstract:

The Smooth Decomposition (SD) is a statistical analysis technique for finding structures in an ensemble of spatially distributed data such that the vector directions not only keep the maximum possible variance but also the motions, along the vector directions, are as smooth in time as possible. The notion of the dual smooth modes is introduced and used in the framework of oblique projection to expand a random response of a system. The dual modes define a tool that transforms the SD in an efficient modal analysis tool. The main properties of the SD are discussed and some new optimality properties of the expansion are deduced. The parameters of the SD give access to modal parameters of a linear system (mode shapes, resonance frequencies and modal energy participations). In case of nonlinear systems, a richer picture of the evolution of the modes versus energy can be obtained analyzing the responses under several excitation levels. This novel analysis of a nonlinear system is illustrated by an example.

Ville Kolehmainen (University of Eastern Finland) VILLE.Kolehmainen@uef.fi

Approximation Errors, Inverse Problems and Model Reduction

Abstract:

The approximation error approach was proposed in [J. Kaipio & E. Somersalo, Statistical and Computational Inverse Problems, Springer, 2004] for handling modelling errors due to model reduction and unknown nuisance parameters in inverse problems. In this talk, we discuss the application of the approximation error approach for approximate marginalization of modelling errors caused by inaccurately known sensor parameters in diffuse optical tomography. We also describe how the approximation error model can be employed for construction of surrogate models for computer simulations.

Zbigniew Bulinski (Silesian University of Technology) zbigniew.bulinski@polsl.pl

Application of the Proper Orthogonal Decomposition for Bayesian Estimation of flow parameters in porous medium

Abstract:

The porous medium is a solid material (solid matrix) containing interconnected voids which might be partially or fully filled with a fluid. This definition includes a wide range of substances used in the modern industry, as well as encountered in nature, starting from materials like: sand, different types of rock, soil, wood, living tissue and artificial (manmade) porous materials like: metal or ceramic foams, building materials (brick, concrete etc.), insulating materials (mineral or glass wool, polystyrene foam etc.). The widespread occurrence of porous materials in every-day life and their interesting properties are causing intensive research in this subject. Parameters describing flow through porous materials, like porosity, pore diameter, permeability, tortuosity, etc., are of special interest. This paper deals with the Bayesian estimation of chosen flow parameters in a porous material based on pressure drop measurements. In order to decrease the computational time necessary to generate an ergodic Markov Chain, Proper Orthogonal Decomposition was used to construct off-line, low order approximation of the porous media flow problem. This model was further coupled with the Metropolis-Hastings algorithm to retrieve the posterior distribution of unknown parameters.