Pan-American Workshop 2018

June 11-15, 2018

EVENT KEY:

Invited Talk	Short Presentation	Mini Workshop	Poster Presentation

TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
7:00 AM					
7:30 AM	Registration				
8:00 AM					
8:30 AM	Welcome	Registration	Registration	Registration	
9:00 AM	Invited 1	Invited 3	Invited 2	Invited 6	
9:30 AM					
10:00 AM	Coffee	Coffee	Coffee	Invited 7	
10:30 AM	ST 32	ST 30	ST 4		
11:00 AM	ST 18	ST 31	ST 9	Coffee	
11:30 AM	ST 13	ST 7	ST 14	ST 16	
12:00 PM	Lunch	Lunch	Lunch	ST 19	
12:30 PM				ST 3	
1:00 PM				Lunch	
1:30 PM					
2:00 PM	Invited 5	Invited 4	ST 24	ST 8	
2:30 PM			ST 11	ST 10	
3:00 PM	WS 1-26	ST 21	ST 2	ST 12	
3:30 PM	WS 2-27	ST 23	ST 25	ST 17	
4:00 PM	Coffee	Coffee	Coffee	Coffee	
4:30 PM	WS 3-22	ST 37	ST 29	ST 15	
5:00 PM		Posters	ST 20	ST 36	
5:30 PM			ST 35		
6:00 PM	Cocktail		ST 5	Dinner &	
6:30 PM	Reception			Awards	
7:00 PM				Banquet	

Pan-American Workshop 2018

Monday - June 11, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
7:30 AM	8:30 AM	Registration			
8:30 AM	9:00 AM	Welcome			
9:00 AM	10:00 AM	Invited Talk 1	Mimetic Finite Difference Operators & High Order Numerical Quadratures	**Jose E. Castillo** San Diego State University	Mimetic finite difference operators, D and G are discrete analogs of their continuous divergence and gradient operators. These discrete operators satisfy in the discrete sense the same properties that their continuum counterpart ones do. In particular, they satisfy a discrete extended Gauss divergence theorem. We present high order numerical quadrature, associated with the fourth and sixth order mimetic finite difference operators and show that they satisfy the divergence theorem. In addition, we present the extension to curvilinear coordinates. Some examples to illustrate our results are presented that clearly confirm our theoretical results.
10:00 AM	10:30 AM	Coffee Break			
10:30 AM	11:00 AM	Short Presentation 32	Simulations of Ultrasonic Propagation in Bypass Blood Flow	**Eduardo Moreno Hernández** Instituto de Cibernética, Matemática y Física	Ischemia cardiopathy is one of the principal causes of dead in many countries. This disease is caused by an abnormal conditions of the coronary arteries. As a consequence the heart muscle does not receive enough blood for its correct functionality. One of the medical solutions is bypass coronary surgery, where a graft is implanted parallel to the coronary arteries. Normally the blood flow in the implant should be measured during the surgery and the ultrasonic transit time flow method (TTFM) is one with the best performance for this flow measurement. The aim of this study is to carry out the simulation of the flow in the bypass using Finite Element Methods, which includes the ultrasonic pulse propagation through this flow. The simulations assume viscoelastic properties for the blood and mechanical properties of the bypass. Piezoelectric material are also included in the model of the TTFM transducer. Different conditions of the transducer and the blood flow are analyzed and presented. Several differential equations are presented from Navier Stoke for the blood flow to the wave and piezoelectric equations for the TTFM transducers. Comsol software 5.2 is used to solve the PDE and the performance of different numerical solvers is studied.

Pan-American Workshop 2018

Monday - June 11, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
11:00 AM	11:30 AM	Short Presentation 18	Sparse Coding: Theory, Implementation and a Practical Problem	**Valia Guerra Ones** Technical University of Delft	In a wide range of applications, a very useful strategy consists of representing a signal as a linear combination of basis vectors. While techniques such as Principal Component Analysis or Wavelet transformation involve a complete set of basis vectors, Sparse Coding discovers an over-complete bases, termed Dictionary, finding succinct representations (most of the coefficients are zero) of the signal. In this work, we discuss theoretical aspects, formulations and computational algorithms of Sparse Coding and its application in a practical problem: Super-resolution (SR) or Image scale-up problem. Our main contribution is proposing a novel approach for solving the SR problem using Sparse Coding in the multi-frame case. The main idea is introducing a group-of-pictures (GOP) structure and detecting static and moving parts of the GOP. Then we super-resolve the low rank frame and sparse frames separately using Sparse Coding. The proposed strategy results in significant time reductions. Experimental evaluations are shown. Finally, we discuss some aspects about Convolutional Sparse Coding.
11:30 AM	12:00 PM	Short Presentation 13	An Efficient Preconditioning Method for Ill-Conditioned Linear Systems	**Takeshi Ogita** Tokyo Woman's Christian University	This study aims to compute accurate numerical solutions of ill-conditioned linear systems. For this purpose, several preconditioning methods have been developed. Using such preconditioning methods, the condition number of the coefficient matrix can be reduced efficiently, and an accurate solution of the linear system can be obtained. However, the computational cost for such preconditioning methods is considerably larger than the standard numerical algorithm, such as LU factorization, in ordinary floating-point arithmetic, since some matrix multiplication in higher-precision arithmetic is required. In this study, we modify this point by exploiting the structure of the coefficient matrix, and develop an accurate and efficient algorithm for solving ill-conditioned linear systems. As a result, the computational cost for the preconditioning can significantly be reduced with similar quality to the previous methods.
12:00 PM	2:00 PM	Lunch Break			

Pan-American Workshop 2018

Monday - June 11, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
2:00 PM	3:00 PM	Invited Talk 5	Reaction-Diffusion Models: Dynamics and Control	**Enrique ZuaZua** Deustotech-Bilbao, UAM-Madrid & LJLL-UPMC-Paris	Reaction-diffusion equations are ubiquitous and its applications include combustion and population dynamics modelling. There is an extensive mathematical literature addressing the analysis of steady state solutions, traveling waves, and their stability, among other properties. Control problems arise in many applications involving these models. And, often times, they involve control and/or state constraints, as intrinsic requirements of the processes under consideration. In this lecture we shall present the recent work of our team on the Fisher-KPP and Allen-Canh or bistable model. We show that these systems can be controlled fulfilling the natural constraints if time is large enough. This is in contrast with the unconstrained case where parabolic systems can be controlled in an arbitrarily small time, thanks to the infinite velocity of propagation. The method of proof combines various methods and, in particular, employs phase-plane analysis techniques allowing to build paths of steady-state solutions. The control strategy consists then in building trajectories of the time-evolving system in the vicinity of those paths. We shall conclude our lecture with a number of challenging open problems.
3:00 PM	3:30 PM	Mini-Workshop 1-26	Producing Divergence Free Approximations to Incompressible Flows	**Johnny Guzman** Brown University	Finite element methods are widely used in approximating incompressible flows. However, most methods produce discrete velocity fields that are NOT divergence free although this property is desirable. In this talk, we discuss the obstacles in producing stable and divergence free producing numerical methods. We then show several examples of methods that achieve this. This is joint work with Michael Neilan and Ridgway Scott.
3:30 PM	4:00 PM	Mini-Workshop 2-27	Optimal Control of MANF to Prevent Apoptosis in Retinitis Pigmentosa	**Luis Melara** Shippensburg University	Protein misfolding is one of the major causes of apoptosis in Retinitis Pigmentosa, where apoptosis is programmed cell death. Mesencephalic-Astrocyte-derived-Neurotrophic Factor (MANF) is a protein that has been shown to correct protein misfolding, thus reducing the death of cells due to “cell suicide." In this talk, we formulate an optimal control problem hat incorporates MANF treatment to rescue photoreceptors in the eye. Numerical results are shown and discussed.
4:00 PM	4:30 PM	Coffee Break			

Pan-American Workshop 2018

Monday - June 11, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
4:30 PM	5:00 PM	Mini-Workshop 3-22	CutFEM for Fluid-Structure Interaction Problems	**Marcus Sarkis** Worcester Polytechnic Institute	Interface problems arise in several applications including heart models, cochlea models, aquatic animal locomotion, blood cell motion, front-tracking in porous media flows and material science, to name a few. One of the difficulties in these problems is that solutions are normally not smooth across interfaces, and therefore standard numerical methods will lose accuracy near the interface unless the meshes align to it. However, it is advantageous to have meshes that do not align with the interface, especially for time dependent problems where the interface moves with time. Remeshing at every time step can be prohibitively costly, can destroy the structure of the mesh, can deteriorate the well conditioning of the stiffness matrix, and affect the stability of the problem. In this talk we present finite element methods for solving interface problems where the finite element triangulation does not fit the interface. We discuss methods for Stokes interface problems and fluid-structure interactions. This is a joint work with my PhD student Kyle Dunn.
6:00 PM		Cocktail Reception			

Pan-American Workshop 2018

Tuesday - June 12, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
8:30 AM	9:00 AM	Registration			
9:00 AM	10:00 AM	Invited Talk 3	50 (+) Years of Numerical Analysis: A Personal View	**Victor Pereyra** Stanford University & San Diego State University	In this talk I will touch briefly on five different subjects that stem from my 10 most cited papers spanning 43 years, namely: Variable Projections (VARPRO), fast Vandermonde solvers and multidimensional polynomial approximation (VANDER), deferred corrections (PASVA series), seismic ray tracing (RAY3D, TERRASA) and least squares data fitting (book). The names in parenthesis correspond to public domain software associated with the topic.
10:00 AM	10:30 AM	Coffee Break			
10:30 AM	11:00 AM	Short Presentation 30	Functional Data Analysis Applied to a Study of Mexican Leading Companies	**Cristina O. Chávez-Chong** ICIMAF, Cuba	Functional data analysis has become an important field of research in Statistics in the last years. This presentation shows a combination of Functional Principal Component Analysis and Functional Canonical Correlation Analysis in a study of economic data in order to establish a relationship between job generation, firm size, and actives in a group of leading Mexican companies.
11:00 AM	11:30 AM	Short Presentation 31	Subdivision Based Snakes for Contour Detection	**Victoria Hernández Mederos** Instituto de Cibernética, Matemática y Física	In this talk we propose a method for computing the contour of an object in an image using a snake represented as a subdivision curve. The evolution of the snake is driven by its control points which are computed minimizing an energy that pushes the snake towards the boundary of the interest region. Our method profits from the hierarchical nature of subdivision curves, since the unknowns of the optimization process are the few control points of the subdivision curve in the coarse representation and, at the same time, good approximations of the energies and their derivatives are obtained from the fine representation.
11:30 AM	12:00 PM	Short Presentation 7	Dispersive Effects for Nonlinear Waves in Periodic Media	**David I. Ketcheson** King Abdullah University of Science & Technology	Hyperbolic PDE models like those of shallow water waves or nonlinear elastic waves generically lead to shock formation or wave breaking. These systems do not describe dispersive waves, but dispersive effects can arise in such systems as a result of periodically- or randomly-varying coefficients or ambient state. Effective dispersion can arise due to both reflection and diffraction of waves, and it can drastically alter the long-term evolution of solutions, for instance by leading to solitary waves or by destabilizing shock waves. I will review what is known about these effects and some open questions.
12:00 PM	2:00 PM	Lunch Break			

Pan-American Workshop 2018

Tuesday - June 12, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
2:00 PM	3:00 PM	Invited Talk 4	Stimulation of Carbonate Mineralization During Carbon Sequestration Through Excess Alkalinity Aquired from Algal Production Pond (APP) Supernatant	**Christopher Paolini** San Diego State University	Algal Production Ponds (APP) used for algae biofuel generation require a source of CO2 for photosynthesis, a process that produces hydroxide ions (OH-) during carbohydrate reactions. The abundance of hydroxide ions can increase pond water pH to 10 or greater and provides a source of alkalinity, in addition to a mechanism for both CO2 disposal and biofuel generation. Approximately 900 billion gallons of formation water are produced each year during Enhanced Oil Recovery (EOR) operations in the United States. Produced water is typically injected back into disposal wells at a significant cost to the oil and gas producer. A synergistic process is presented that uses produced water and recovered CO2 for algae growth in APPs, and the high-pH, high-saline supernatant as a source of excess alkalinity for enhanced carbonate mineralization in deep geologic formations. We present a 3D Thermal-Hydrologic-Mechanical-Chemical ("THMC") application for modeling geologic CO2 sequestration and waste water injection in brine saturated sandstone-shale reservoirs, and investigate the effects of alkaline waste water injection, following CO2 injection, on carbonate mineral saturation and precipitation, under variable injection temperatures and pressures. A nine-mineral kinetic mechanism governing the dissolution of quartz, potassium feldspar ("K-spar"), anorthite, albite, calcite, kaolinite, smectite, illite, and halite in a porous medium is used, with the aqueous phase pore water temperature modeled using a transient heat advection-diffusion transport model with non-constant thermal coefficients. Water-rock interaction is coupled with a transient mixed finite element method for fluid pressure and velocity, and a Galerkin method for poroelastic mechanics. Thermal coefficients (specific heat and specific enthalpy) are temperature and pressure dependent and computed using the revised Helgeson-Kirkham-Flowers ("HKF") model for approximating the thermodynamic properties of aqueous electrolytic solutions under high temperature and high-pressure. The HKF derived heat capacity and enthalpy of charged aqueous species arising from the interaction of CO2-rich brine with sandstone are used in a heat transfer model source term for computing the aqueous phase volumetric energy generation rate. The poroelastic and pressure-velocity fields are solved in parallel with MPI using domain decomposition. Numerical simulations demonstrate the feasibility of inducing carbonate mineral formation through alkaline waste injection following CO2 injection.
3:00 PM	3:30 PM	Short Presentation 21	Considerations on the Magnitude of the Shift in the Shifted Laplace Preconditioner for the Helmholtz Equation Combined with Deflation	**Domenico Lahaye** DIAM - TU Delft	In recent work we showed that the performance of the complex shifted Laplace preconditioner for the discretized Helmholtz equation can be significantly improved by combining it multiplicatively with a deflation procedure that employs multigrid vectors. In this contribution we argue that in this combination the preconditioner improves the convergence of the outer Krylov acceleration through a new mechanism. This mechanism allows for a much larger damping and facilitates the approximate solve with the preconditioner. The convergence of the outer Krylov acceleration is not significantly delayed and occasionally even accelerated. To provide a basis for these claims, we analyze for a one-dimensional problem a two-level variant of the method in which the preconditioner is applied after deflation and in which both the preconditioner and the coarse grid problem are inverted exactly. We show that in case that the mesh is sufficiently fine to resolve the wave length, the spectrum after deflation consists of a cluster surrounded by two tails that extend in both directions along the real axis. The action of the inverse of the precondioner is to shrink the length of the tails while at the same time rotating them and shifting the center of the cluster towards the origin. A much larger damping parameter than in algorithms without deflation can be used.

Pan-American Workshop 2018

Tuesday - June 12, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
3:30 PM	4:00 PM	Short Presentation 23	An Application of the Woodbury Formula to Monte Carlo Simulation of a Random Coefficient One Dimensional Pressure Equation	**O. Andrés Cuervo** Universidad Nacional de Colombia	In this paper we consider the one dimensional pressure equation with random coefficients. The problem is approximated by a piecewise continuous and linear finite element method. In this is common practice to use classical Monte Carlo approach to compute approximations of the mean value of the solution. In the classical Monte Carlo method, samples of the coefficient are generated and for each sample, a finite element approximation is computed. We propose a new strategy that speeds up Monte Carlo approximation of the mean value of the solution. The new strategy uses a Woodbury formula that allows us to implement an algorithm that needs two LU factorizations in a preprocessing step instead of one LU factorization of each sample. We present the motivations and design of the method as well as numerical test to show its performance in comparison with classical Monte Carlo approach.
4:00 PM	4:30 PM	Coffee Break			
4:30 PM	5:00 PM	Short Presentation 37	Parallel Adaptive and Robust Multigrid Methods	**Gabriel Wittum** KAUST, ECRC	Numerical simulation has become one of the major topics in Computational Science. To promote modelling and simulation of complex problems new strategies are needed allowing for the solution of large, complex model systems. Crucial issues for such strategies are reliability, efficiency, robustness, usability, and versatility. After discussing the needs of large-scale simulation we point out basic simulation strategies such as adaptivity, parallelism and multigrid solvers. To allow adaptive, parallel computations the load balancing problem for dynamically changing grids has to be solved efficiently by fast heuristics. These strategies are combined in the simulation system UG ("Unstructured Grids") being presented in the following.
5:00 PM	7:00 PM	Poster Presentations	Remote Sensing Tools Applied to the Spatial Dynamics of the Shoreline of the Rancho Luna Beach, Cuba, Cienfuegos	**Laura Castellanos Torres** Centro de Estudios Ambientales de Cienfuegos (CEAC)	Analysis of the spatial behavior of the coastline of the Rancho Luna beach, in the province of Cienfuegos, Cuba; through the application of remote sensing and SPOT images, in the period studied 2004 -2014.

Pan-American Workshop 2018

Tuesday - June 12, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
			Mathematical Modeling of Crowd Evacuation from Bounded Domains	**Damian Knopoff** Universidad Nacional de Cordoba - CONICET	A mathematical model of the evacuation of a crowd from bounded domains is derived by a hybrid approach with kinetic and macro features. Interactions at the micro-scale, which modify the velocity direction, are modeled by using tools of game theory and are transferred to the dynamics of collective behaviors. The velocity modulus is assumed to depend on the local density. The modeling approach considers dynamics caused by interactions of pedestrians not only with all the other pedestrians, but also with the geometry of the domain, such as walls and exits. Interactions with the boundary of the domain are non local and described by games. Numerical simulations are developed to study evacuation time depending on the size of the exit zone, on the initial distribution of the crowd and on a parameter which weighs the unconscious attraction of the stream and the search for less crowded walking directions.
			Characteristic Behaviour of Models of Fluid Flow in Porous Media	**Luis Xavier Vivas Cruz** Centro de Ingeniería y Desarrollo Industrial, CIDESI	Generalizations of the Warren and Root model are presented. With this goal, recharge of fluid at the external boundary, telegraphic effect, and anomalous behavior of different flow regime are independently considered. A classification of the characteristic behaviour of the solutions of each of these models is made. Our solutions contemplate the known behavior at limit cases already found in the literature, and in addition, a matching between the exact and numerical solutions is presented.

Pan-American Workshop 2018

Tuesday - June 12, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
			Data-Driven Distributionally Robust Optimization Applied to Probability Density Estimation and Portfolio Optimization	**Diego Fernando Fonseca Valero** Universidad de los Andes	In the field of mathematical optimization, stochastic programming is a framework for modeling optimization problems that involves uncertainty in the form of a random variable. Usually, the probability distribution of the variable is unknown, hence another approach known as Distributionally Robust Optimization (DRO) has emerged recently. This approach assumes that the true distribution of the random variable involved in the problem belongs to a set of distributions called Ambiguity Set. Therefore, every stochastic optimization problem has its DRO counterpart. When this set is defined as a ball with respect to the Wasserstein metric centered at the empiric distribution, the DRO problem can be reformulated as a semi-infinite optimization problem and, depending on the objective function, this problem can be formulated as a finite convex optimization problem. There are several fields in which stochastic optimization problems appear, in this work we show two applications. First, in the context of statistics, it is known that a way to estimate the probability density function of a random variable is the kernel density estimation (KDE). The estimator that the method produces depends on a parameter known as bandwidth, which is obtained by minimizing an expression known as MISE (Mean Integrated Squared Error). We show that this minimization problem is in fact a stochastic problem and its DRO version is formulated. This allows to choose the optimal bandwidth without assuming conditions on the density function that we wish to estimate. Finally, a DRO version of the portfolio optimization problem is exhibited in the context of the Markowitz Mean-Variance Portfolio Theory. Here, we wish to find the portfolio that minimizes the variance subject to the expected return being greater than an amount established by the investor. In practice the returns are random and its distribution is unknown and therefore sample estimations are used for the mean vector and the covariance matrix providing solutions highly sensitive to the sample. We show that this phenomenon is reduced with our method. Keywords: Robust Optimization, Wasserstein metric, portfolio optimization, density estimation.

Pan-American Workshop 2018

Wednesday - June 13, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
8:30 AM	9:00 AM	Registration			
9:00 AM	10:00 AM	Invited Talk 2	A Least-Squares Approach To Two-Fluid Electromagnetic Plasma	**Thomas A. Manteuffel** University of Colorado Boulder	A two-fluid plasma (TFP) model is presented, both as a stand-alone solver and as the preconditioner to a fully implicit, particle-in-cell (PIC) simulation. The model couples fluid conservation equations for ions and electrons to Maxwells equations. A Darwin approximation of Maxwell is used to eliminate spurious light waves. After scaling and modification, the TFP-Darwin model yields a nonlinear, first-order system of equations whose Frechet derivative is shown to be uniformly H1-elliptic. This system is addressed numerically by nested iteration (NI), a First-Order System Least Squares (FOSLS) discretization, adaptive local mesh refinement, and scaled AMG system solver. Numerical tests demonstrate the efficacy of this approach, yielding an approximate solution within discretization error in a relatively small number of computational work units.
10:00 AM	10:30 AM	Coffee Break			
10:30 AM	11:00 AM	Short Presentation 4	Discrete Mollification of a Mimetic Explicit Scheme for One-Dimensional Convection Diffusion Equations	**Deyanira Maldonado Guerrero** Escuela de Matemáticas, Universidad Industrial de Santander, Santander, Colombia	In this paper is presented the discrete mollification of an explicit time-stepping mimetic scheme for partial differential equations. It considers the discrete mollification of gradient and divergence operators involved in the standard mimetic scheme. In addition, numerical test problems show this new scheme produces better approximations than the mimetic scheme.
11:00 AM	11:30 AM	Short Presentation 9	New Analysis of Characteristics-Mixed FEMs for Miscible Displacement in Porous Media	**Weiwei Sun**	The method of characteristics type is especially effective for convection-dominated diffusion problems. Due to the nature of characteristic temporal discretization, the method often allows one to use a large time step in many practical computations, while all previous theoretical analyses always required certain restrictions on the time stepsize. In this talk, we present our recent work on establishing unconditionally optimal error estimates for modified methods of characteristics for N-S equations and miscible displacement problem. For this purpose, we introduce a characteristic time-discrete system. We prove that the L^2 error bound of the fully discrete method of characteristics to the time-discrete system is \\$tau$-independent and the numerical solution is bounded in $W^{\{1,\backslash infty\}}$-norm unconditionally. With the boundedness, optimal error estimates are established in a traditional manner. Numerical results confirm our theoretical analysis and clearly show the unconditional stability.

Pan-American Workshop 2018

Wednesday - June 13, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
11:30 AM	12:00 PM	Short Presentation 14	Adaptivity in Mimetic Schemes: Implementation in Convection-Diffusion Problems	**Jorge Villamizar-Morales** Universidad Industrial de Santander, UIS, Colombia/ Universidad de Los Andes, ULA, Venezuela	We present a *h* -adaptive process that defines an optimal mesh to calculate the approximate solution in convection-diffusion diffusion problems by using mimetic numerical methods. The error estimate in the spatial variable is made from the discrete version of the gradient operator. The numerical experiments show the good behavior of this procedure.
12:00 PM	2:00 PM	Lunch Break			
2:00 PM	2:30 PM	Short Presentation 24	On a Goal-Oriented Formulation for Constructing Optimal Reduced-Order Models with Respect to Quantities of Interest	**Serge Prudhomme** Ecole Polytechnique Montréal	The subject of the talk will be concerned with the a mathematical formulation for constructing reduced-order models tailored for the approximation of quantities of interest. The main idea is to formulate a minimization problem that includes an equality or inequality constraint on the error in the goal functional so that the resulting model is capable of delivering predictions of the quantity of interest within some prescribed tolerance. The formulation will be applied and tested to the so-called Proper Generalized Decomposition (PGD) method. Such a paradigm represents a departure from classical goal-oriented approaches in which a reduced model is first derived by minimization of the energy, or of residual functionals, and then adapted via a greedy approach by controlling the error with respect to quantities of interest using dual-based error estimates. Numerical examples will be presented in order to demonstrate the efficiency of the proposed approach. In particular, we will consider the case of a delaminated composite material simulated in terms the Proper Generalized Decomposition approach.
2:30 PM	3:00 PM	Short Presentation 11	Clathrate Hydrates: Applied to Hydrogen Storage	**Daniel Porfirio Luis Jimenez** CIDESI	Since the discovery of clathrate hydrate of hydrogen in 2002, many efforts have been done to study this compound in many scientific areas. In the present work we show some recent discoveries made with molecular dynamics simulations in order to observe the capability of clathrate hydrates to store hydrogen molecules; after that, the stability of hydrogen clathrate hydrate was investigated using a classical molecular dynamics calculation package “Gromacs”, arranging only one hydrogen molecule into each host frame of the hydrogen clathrate. Coordination number was evaluated to be used as stability criteria of the clathrate structure. The diffusion coefficient of the hydrogen molecules was calculated to observe how the movement of the H2 molecules can affect the stability of the structure. These calculations were done with a NPT ensemble at a series of temperatures from 220 to of 250 K and at different pressures. TIP4P/Ice potential was used for water molecules and a potential that consists in three sites of partial charges and a Lennard-Jones site for the molecules of hydrogen.

Pan-American Workshop 2018

Wednesday - June 13, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
3:00 PM	3:30 PM	Short Presentation 2	Topological Description of the Complex Flow Field in Cerebral Aneurysms	**Simona Hodis** Texas A&M University - Kingsville	Ruptured aneurysms are known to have complex flow patterns and concentrated inflow jet, but a quantifiable measure of the degree of complexity in patient-specific geometries has not been established. The purpose of this study is to provide an analytic solution for calculating the flow complexity parameter based on the curvature and torsion of the flow field. Analyzing the flow complexity parameter in the jet and non-jet regions inside the aneurysm dome, we found that on average, in a ruptured case the jet region is significantly less complex (4.5 times) than the jet region in an unruptured case, while the non-jet region is significantly more complex (3.5 times) than the non-jet region in an unruptured case. We also found a strong positive correlation of the non-jet complexity with the dome volume in ruptured cases, but no correlation between jet complexity and the dome volume. These findings suggest that a ruptured aneurysm has more than four times more concentrated inflow jet and more than three times more complex flow patterns in non-jet region than an unruptured aneurysm.This newly implemented kinematic parameter provides a measurable degree of complexity of flow patters in cerebral aneurysms that can better assess aneurysm rupture risk.

Pan-American Workshop 2018

Wednesday - June 13, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
3:30 PM	4:00 PM	Short Presentation 25	Energy Management System for an Electric Vehicle with Batteries and Ultracapacitors Applying Model Predictive Control and Short Term Predictive Power Demand	**Maximiliano Asensio** Grupo de Electrónica Aplicada (GEA)	In pure electric vehicles (VEs), the bank of batteries is the main energy storage element, while the simplest possible hybridization involving a complementary storage element is made by including ultracapacitors (UCs). Batteries are elements capable of delivering energy at a slow rate but during long periods of time (high energy density). In a complementary form, UCs can efficiently deliver large quantities of energy in a short time (high power density). Hence, this complementariness not only enhances the vehicle response to peak power requirements but also contributes to preserve the batteries, which constitutes one of the most important elements of the vehicle cost. In order to efficiently operate these vehicles, it is then necessary to determine the instantaneous power split between these two storage elements in such a way that they satisfy the power required by the vehicle, which is unknown a priori, and use each element according to its capability. In this work we present a power split strategy, based in non-linear model based predictive control (NMPC). In this approach a cost function is proposed in order to pursue two objectives: minimizing the battery current fluctuation, so preserving its health, and regulating the UC voltage to a desired reference value. The NMPC scheme involves the solutions of successive constrained optimal control problems over what is known as receding horizon. These finite horizon control problems are solved by modeling the system, discretizing it in time and then successively minimizing the cost function using a non-linear programming tool. As it is necessary to perform a prediction of the unknown power demand over each sliding interval, and this interval is a short time ahead for this application, a simple predictive autoregressive model is proposed. Simulation results are presented and compared with the ideal case in which the future information of the power requirement is completely known. The control strategy produces a smooth battery current avoiding its degradation and ageing while UCs contribute with the remaining required power, maintaining its state of charge within the established working range.
4:00 PM	4:30 PM	Coffee Break			
4:30 PM	5:00 PM	Short Presentation 29	Analysis of Publication Activity of Macrobrachium using Topological Data Analysis	**Guillermo Aguirre Carrazana** University of Havana	In this work we use the simplicial complex approach to word co-occurrences, which provides a natural framework for the study of higher-order relations in the space of scientific knowledge. Using topological and statistical methods we explore the landscape of scientific research around Macrobrachium.
5:00 PM	5:30 PM	Short Presentation 20	Error Analysis of Splitting Methods for Semilinear Evolution Equations	**Takiko Sasaki** Meiji University	We consider a Strang-type splitting method for an abstract semilinear evolution equation *¥partial_t u= Au+F(u)* . Roughly speaking, the splitting method is a time-discretization approximation based on the decomposition of operators A and F. Particularly, the Strang method is a popular splitting method and is known to be convergent at a second order rate for some particular ODEs and PDEs. In this talk, we propose a generalization of the Strang method and prove that our proposed method is convergent at a second order rate.

Pan-American Workshop 2018

Wednesday - June 13, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
5:30 PM	6:00 PM	Short Presentation 35	Investigation of the Coefficient of Friction in the Lubricated Contact Between Roughness and Rigid Plane via MEF	**Marcus Vinicius de Souza Ferraz** Universidade Federal de Juiz de For a	The knowledge of the topography of surfaces and an understanding of the interaction between them is essential for any study involving the phenomena of friction, wear and lubrication. The study of the relationship between friction and roughness parameters is a difficult problem of both industrial and academic interest and experimental and theoretical works have shown that a fluid film between two rough surfaces in relative motion prevents solid - solid contact and can provide very low friction and negligible wear. The mathematical modeling used in this paper is based on classical models, such as the Reynolds equation for the description of the hydrodynamic phenomena and the formulations of Hertz (1896) and Greenwood and Williamson (1966) of the contact between the asperities of rough surfaces. To address the complexity of the interactions between the fluid and the contacted solid pairs, the Lagrangian-Eulerian Arbitrary description is presented in this research. Through the Finite Element Method, a three-dimensional model is generated in Abaqus to identify contact pressures, resulting tangential and normal stresses, and friction coefficients resulting from sliding between a textured and lubricated surface and a rigid plane (in analogy to classic contact models), whose roughness profiles are constructed from information on the quadratic roughness of dental surfaces. The sensitivity of some lubricant parameters in the determination of the coefficient of friction is also evaluated and models with different boundary conditions are proposed. A methodology proposed here emerges as an effective alternative in the field of Tribology, in the prediction of the coefficient of friction and other relevant variables to a phenomenon still little understood. A sensitivity analysis of the modeling parameters is performed, in order to identify how they considerably affect the mechanical behavior at the contact interface.
6:00 PM	6:30 PM	Short Presentation 5	Bayesian Solutions for Inverse Problems	**Ali Mohammad-Djafari** CNRS	In this presentation, two inverse problems in imaging are considered: the first a linear inverse problem of computed tomography (CT) and the second the bilinear inverse problem of diffraction tomography (DT). For both cases, a hierarchical prior model, appropriate for piecewize homogeneous objects, which are usual in non destructive testing (NDT) imaging applications, is proposed. This model is called Gauss-Markov-Potts. Then, the Bayesian inference approach is used to obtain the expression of the joint posterior law of all the unknowns given the data. Finally, approximate Bayesian computation (ABC) and in particular the variational Bayesian approximation (VBA) is used to propose computationally scalable reconstruction algorithms. Some simulation and real data results are provided.

Pan-American Workshop 2018

Thursday - June 14, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
8:30 AM	9:00 AM	Registration			
9:00 AM	10:00 AM	Invited Talk 6	Residence Times of Cienfuegos Bay	**Alain Muñoz Caravaca** Centro de Estudios Ambientales de Cienfuegos	A high-resolution numerical model was applied to analyze the hydrodynamical exchange processes of the Cienfuegos Bay with the Caribbean Sea. Results show that freshwater inputs and wind are the main factors controlling the water exchange in the bay. Nine simulation case studies with three wind conditions and three freshwater inputs were carried out. The main conclusion is that the Cienfuegos Bay system has a slow exchange rate, with an average flushing time of 39 days during the rainy period and 50 days during the dry one, for the most probable wind direction. Two new temporary scales for Cienfuegos Bay are discussed: the local e-flushing time and the flushing lag. The results obtained for these new variables validate the slow exchange capacity of the bay.
10:00 AM	11:00 AM	Invited Talk 7	Numerical Weather Prediction at the Cuban Meteorological Service	**Ida Mitrani Arenal** Centro de Fisica de la Atmosfera/ Instituto de Meteorologia	A description of the historical development of the numerical weather prediction in the Cuban Meteorological Service is presented. The advantages and limitations on the application of numerical modeling in Cuba are briefly explained. It is described the chain of models that are used at the current time in the operative weather forecast. The main forecasting tacks have been: Hurricane tracks, wind waves, sea level rise due to meteorological events, coastal floods, intense rains and strong winds. However, in the last five years, the sea water temperature, the salinity and the marine stream components have been added to de set of forecast variables. It concludes that the quality of the operative weather forecast has increased, due to the efficient use of numerical modeling.
11:00 AM	11:30 AM	Coffee Break			
11:30 AM	12:00 PM	Short Presentation 16	Mathematical Procedures to Solve Fluid Flow Model in Porous Media	**Alfredo González-Calderón** CIDESI	New solutions of fluid flow models with application in test well or pumping wells are presented: Transform integral solutions for double-porosity reservoirs with fluid recharge at the external boundary, contour integral solution of a telegraphic Warren and Root model, and variable separation solution of the Warren and Root model. In addition, exact solutions in Laplace space of anomalous fluid flow models are given. In these latter proposals, a generalized Cattaneo equation is used in order to describe the transition of solutions between their elliptic, parabollic, and hyperbolic behaviors.

Pan-American Workshop 2018

Thursday - June 14, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
12:00 PM	12:30 PM	Short Presentation 19	Non-Conforming fe/be Coupling for a Two-Dimensional Electromagnetic Problems	**Jorge Ospino** Universidad del Norte	In this work we present a non-conforming finite element/boundary element coupling method to solve the two-dimensional electromagnetic problem for the time harmonic Maxwells equations. Here we combine the approach by Brenner et al. [1, 2, 3] for the fem part with the approach by Carstensen and Funken [4] for the fem/bem coupling. We present numerical simulations which show the effectiveness of our non-conforming fem/bem coupling. Key words: Non-conforming fe/be coupling, electromagnetic problem, eddy current problem. References [1] S. C. Brenner, J. Cui, F. Li, and L. Y. Sung, A nonconforming finite element method for a two-dimensional curl-curl and grad-div problem, Numer. Math., 109 (2008), pp. 509533. [2] S. C. Brenner, F. Li, and L. Y. Sung, A locally divergence-free nonconforming finite element method for the time-harmonic Maxwell equations, Math. Comp., 76 (2007), pp. 573595. [3] S. C. Brenner, F. Li, and L. Y. Sung, A locally divergence-free interior penalty method for two-dimensional curl-curl problems, SIAM J. NUMER. ANAL., 46 (2008), pp. 11901211. [4] C. Carstensen and J. S. A. Funken, Coupling of non-conforming finite elements and boundary elements I: A priori estimates, Computing. Springer-Verlag, 62 (1999), pp. 229 241.
12:30 PM	1:00 PM	Short Presentation 3	Refined Interlacing Properties for Zeros of Paraorthogonal Polynomials on the Unit Circle	**Kenier Castillo** Centre for Mathematics, University of Coimbra, Portugal	The purpose of this talk is to extend in a simple and unified way the known results on interlacing of zeros of paraorthogonal polynomials on the unit circle. These polynomials can be regarded as the characteristic polynomials of any matrix similar to an unitary upper Hessenberg matrix with positive subdiagonal elements.
1:00 PM	2:00 PM	Lunch Break			
2:00 PM	2:30 PM	Short Presentation 8	Test Matrices for Symmetric Eigenvalue Problems Using Weighing Matrices	**Katsuhisa Ozaki** Shibaura Institute of Technology	This talk concerns test matrices for numerical computations of symmetric eigenvalue problems. If exact eigenvalues are known beforehand, it is useful for checking accuracy and stability of numerical algorithms. We propose methods that produce a matrix with exact eigenvalues using the weighing matrix and error-free transformations of floating- point numbers. The computational cost of the proposed methods is less than or equal to that of a matrix multiplication.

Pan-American Workshop 2018

Thursday - June 14, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
2:30 PM	3:00 PM	Short Presentation 10	Applications of Floating-Point Filters	**Yuki Ohta** Shibaura Institute of Technology	Floating-point numbers and floating-point arithmetic as defined by IEEE 754 are widely used on recent computers. Numerical computations are performed very fast, however, computed results may not be accurate due to accumulation of rounding errors. Therefore, verifying the accuracy of approximate solutions has been frequently discussed. Floating-point filters are one technique in the course of such result verification. For example, floating-point filters can be used to guarantee the sign of a computed result such as the sign of a matrix determinant which is a major task in the field of computational geometry. In this talk we present several applications of floating-point filters. The proposed methods can be used not only for sign verification but also for providing computable absolute and relative error bounds. Our filters are suited for many computational tasks including sum, dot product, evaluation of polynomials, and so forth.
3:00 PM	3:30 PM	Short Presentation 12	Rounding Error Analysis of QR Decomposition Using LU Factors Based on CholeskyQR Algorithm	**Takeshi Terao** Shibaura Institute of Technology	QR decomposition is a decomposition of a matrix into a product QR of an orthogonal matrix Q and an upper triangular matrix R. It is often used in numerical linear algebra. The CholeskyQR algorithm is one of algorithms for QR decomposition and it can be implemented using mainly level 3 routines in BLAS. In addition, there is an advantage in terms of communication avoidance. Therefore, it is suited for computing on distributed memory parallel computers. However, this algorithm cannot be applied for ill-conditioned matrices. We propose a new algorithm for QR decomposition using LU decomposition. In the presentation, we will show results of error analysis of the proposed algorithm, computational performance, and accuracy compared with the original CholeskyQR algorithm.
3:30 PM	4:00 PM	Short Presentation 17	Numerical Approach of Estimating Blow-Up Rate Using the Rescaling Algorithm	**Tetsuya Ishiwata** Shibaura Institute of Technology	In this talk, we focus on the blow-up solutions for a quasilinear parabolic partial differential equation. We propose a numerical method for estimating blow-up rate of blow-up solutions based on the rescaling algorithm and show a mathematical result for this method. Finally we show several examples and numerical observations.
4:00 PM	4:30 PM	Coffee Break			
4:30 PM	5:00 PM	Short Presentation 15	An Iterative Method for a Special Evolution Variant of the Lotka-Volterra System	**Ricardo Cano Macias** Universidad de La Sabana	We propose an iterative method for a kind of Lotka-Volterra system. The method is based on successive substitutions of a linear approximation of the original problem; this approach has the advantage to treat two equations separately in each iteration step. By means of Sobolev embedding and regularity results, we prove that the sequence of weak solutions obtained is a Cauchy sequence that converges to the weak solution of the problem. These results are verified by numerical simulations for different cases of study. In addition, under suitable initial conditions, we construct an invariant region to show the global existence in time of solutions for the system.

Pan-American Workshop 2018

Thursday - June 14, 2018

START	END	TYPE	TITLE	PRESENTER	ABSTRACT
5:00 PM	5:30 PM	Short Presentation 36	Computational Model of Lubricated Contact Between Shaft and Rolling Bearing	**Marvelúcia Silmara Silva Almeida** Universidade Federal de Juiz de Fora	This paper presents the mathematical and computational modeling by Abaqus of the lubricated contact between the rough surface of a rolling bearing and the rigid plane of a shaft. The study of the fluid-structure iteration considered is based on the science called Tribology and on the modeling of the Lagrangian-Eulerian Arbitrary method. The aim is to analyze the relationship between slip friction and wear produced between the asperities of the surfaces according to the lubrication regime used, in order to compare the results obtained by the analysis of the computational model with the ones previously acquired through the bench experiment. The experimental test consists of a torque supply (electric motor), a coupling between the motor shaft and the analysis shaft, which is supported by two rolling bearings and activate a pair of gears. As input data, the geometry and the relative velocities of the movement are obtained, and as outputs, the response in terms of shear stresses is achieved. Initially the tribological pair is considered smooth for comparison with the analytical model based on the rheological equation of Newtonian fluids. Next, the roughness of the bearing surface is included, whose profile is obtained from measurements using a Roughness Meter. According to the measured parameters, probability density functions of the roughness heights are generated, which are discretized in some intervals so that each one represents a main cell of the surface. Thus, by means of homogenization techniques, the relationship of results generated in microscale with those expected in the macroscale is established. Preliminary results demonstrate that the computational model is able to reproduce satisfactorily the planned test.
6:00 PM		Dinner & Awards Banquet			