

VIII Pan-American Workshop Applied and Computational Mathematics

Universidad del Norte » Barranquilla, Colombia
July 21-25, 2014



Financial Markets
Energy and Climate Change
Ocean Sciences
Numerical Analysis
Applied Statistics
Oil Exploration
Seismology

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VIII Pan-American WorkShop: Applied and Computational Mathematics

Program - Monday, July 21, 2014

07:30-10:30	Registration	
08:30-09:30	Welcome	
09:30-10:30	Invited Presentation	
	Room: Auditorium	
	Jose Castillo, San Diego State University <u>Mimetic Discretization Methods</u> <u>Abstract:</u> Mimetic compatible discretizations have been a recurrent theme in the history of numerical methods for solving partial differential equations with variable degree of success. There are many investigations currently active in this area, pursuing different approaches and many algorithms have been developed along these lines. Loosely speaking, "mimetic" or "compatible" algebraic methods have discrete structures that mimic vector calculus identities and theorems. Specific approaches to discretization have achieved this compatibility following different paths, and with diverse degree of generality in relation to the problems solved and the order of accuracy obtainable. Here, we present theoretical aspects of a mimetic method based on the extended Gauss Divergence Theorem as well as examples by means of the Mimetic methods to solve partial differential equations using the Mimetic Library Toolkit (MTK).	
	Short Presentations	
	Room: 22G1	Room: 23G1
10:30-11:00	Second-Order Mimetic Discretization of the Seismic Wave Equation in Heterogeneous Media <i>Freysimar Solano Feo,</i> <i>Universidad Central de Venezuela</i>	Mathematical Modeling of a Direct Bioethanol Pem Fuel Cell <i>R.S. Gomes,</i> <i>Federal University of Rio Grande do Sul</i>
11:00-11:30	Performance Analysis of a Mimetic Finite Difference Scheme for Acoustic Problems: CPU Versus GPU Computing <i>Otilio Rojas,</i> <i>Universidad Central de Venezuela</i>	Development of Reduced Kinetic Mechanisms for Propane and N-Heptane Diffusion Flames <i>R.S. Gomes,</i> <i>Federal University of Rio Grande do Sul</i>
11:30-12:00	Mimetic Discretization of Fourth-Order Hyperbolic Equations on Spatial-Time Staggered Grids <i>Freysimar Solano Feo,</i> <i>Universidad Central de Venezuela</i>	Modeling Supershear Rupture Propagation on Rate and State Faults Accounting for Thermal Pressurization of Pore Fluids <i>Adelis Nieves,</i> <i>Universidad Central de Venezuela</i>

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Program - Monday, July 21, 2014

12:00-14:00	Lunch	
14:00-15:00	Invited Presentation	
	Room: Auditorium	
	Ernst Stephan, Leibniz Universität Hannover <u>hp -Adaptive BEM For Frictional Contact Problems In Linear Elasticity</u> Abstract: A mixed formulation for a Tresca frictional contact problem in linear elasticity is considered in the context of boundary integral equations, which is later extended to Coulomb friction . The discrete Lagrange multiplier, an approximation of the surface traction on the contact boundary part, is a linear combination of biorthogonal basis functions. In case of curved elements, these are the solutions of local problems. In particular, the biorthogonality allows to rewrite the variational inequality constraints as a simple set of complementarity problems. Thus, enabling an efficient application of a semi-smooth Newton solver for the discrete mixed problem, converging locally super-linearly in the frictional case and quadratically in the frictionless case. Typically, the solution of frictional contact problems is of reduced regularity at the interface between contact to non-contact and from stick to slip. To identify the a priori unknown locations of these interfaces two a posteriori error estimations are introduced. In a first step the error is split into specific error contributions resulting from the contact and friction conditions and from the discretization error of a variational equation. For the latter a residual and a bubble error estimation are considered explicitly. The numerical experiments show the applicability of the derived error estimations, in particular in the Coulomb friction case, and the superiority of <i>hp</i>-adaptivity compared to low order uniform and adaptive approaches.	
	Short Presentations	
	Room: 23G1	Room: 24G1
15:00-15:30	Optimally Accurate Mimetic Finite Difference Modeling of Free Surfaces on Elastic Media <i>Luis Cordova,</i> <i>Universidad de Oriente, Venezuela</i>	Analysis of Double Feed Asynchronous Machine in Eolic Generation <i>Patricia Sánchez,</i> <i>Universidad Central de Venezuela</i>
15:30-16:00	Discrete Mollification and the Numerical Solution of Problems Associated to Partial Differential Equations <i>Carlos E. Mejía,</i> <i>Universidad Nacional de Colombia</i>	Numerical Simulation of a Tool to Detect Vulnerable Areas in Case of Tsunamis: A Web Map Service Implementation for Venezuelan Coasts <i>Miguel Rojas,</i> <i>Venezuelan Foundation for Seismological Research</i>
16:00-16:30	Coffee Break	

VIII Pan-American WorkShop: Applied and Computational Mathematics

Program - Monday, July 21, 2014

Short Presentations		
	Room: 23G1	Room: 24G1
16:30-17:00	Applying Mimetic Finite Differences and Model Order Reduction to 2-D Seismic Wave Propagation <i>Otilio Rojas,</i> <i>Universidad Central de Venezuela</i>	Short-Term Load Forecasting Using an Updated Load Curve Formulation <i>Guilherme Guilhermino Neto,</i> <i>Universidade Federal de Juiz de Fora</i>
17:00-17:30	Effect of Wind Direction and Orography on Flow Structures at Baja California Coast: A Numerical Approach <i>Carlos R. Torres,</i> <i>Mexico National Oceanographic Data Center & Institute for Oceanological Research/UABC</i>	On Fractal Dimensions of Natural and Artificial Environments <i>Natalia Naoumova,</i> <i>Pelotas Federal University, Brazil</i>
	Room: 23G1	
17:30-18:00	Building Orthogonal Grids Using Lemniscates <i>Gustavo Adolfo Restrepo,</i> <i>Universidad Nacional de Colombia</i>	

VIII Pan-American WorkShop: Applied and Computational Mathematics

Program - Tuesday, July 22, 2014

07:30-10:30	Registration	
08:30-09:30	Invited Presentation	
	Room: Auditorium	
	Victor Pereyra, Stanford University <u>Seismic Survey Simulation and Imaging in 3D</u> Abstract: Current distributed computing systems allow the simulation of very large seismic surveys consisting of thousands of source-receiver pairs by using the full wave equation. Imaging, such as Reverse Time Migration, also has similar requirements. The clock time required, though, is still fairly significant and it is of interest to see if it can be reduced. In previous work we have shown that Model Order Reduction applied to the 2D acoustic wave equation could produce speed-ups of one order of magnitude when applied to these problems. In principle, there are no conceptual difficulties in extending these techniques to 3D. However, the requirements for existing applications make it more challenging due to the large size simulations involved and the fact that one is restricted to work in a single multicore box for each source-receiver pair. Even with upper end machines, there are difficulties and we will discuss in this talk some proposed alternatives to existing algorithms.	
	Short Presentations	
	Room: 21G1	Room: 22G1
09:30-10:00	On Perturbations of Principal Eigenvalues of Substochastic Matrices <i>Andrei Bouchtein,</i> <i>Pelotas State University, Brazil</i>	A Fuzzy Optimization Model for Berth Allocation Problem to Vessels Arriving with Delay <i>Flabio Gutierrez,</i> <i>Universidad Nacional del Peru</i>
10:00-10:30	Coffee Break	
	Short Presentations	
	Room: 21G1	Room: 22G1
10:30-11:00	On Improving The Block Variable Conjugate Gradient Algorithm <i>Pedro Torres,</i> <i>National University of Asuncion</i>	Comparison of Techniques of Adaptive Penalty on Artificial Bee Colony Algorithm Applied to Optimization Problems in Engineering <i>Grasiele Regina Duarte,</i> <i>Universidade Federal de Juiz e Fora, Brasil</i>

VIII Pan-American WorkShop: Applied and Computational Mathematics

Program - Tuesday, July 22, 2014

	Short Presentations	
	Room: 22G1	
11:00-11:30	Constrained Optimization Framework for 1D Seismic Wave Propagation Problems Anibal Sosa, Universidad Icesi	
	Short Presentations	
	Room: 21G1	Room: 22G1
11:30-12:00	Formal Second-Order Accuracy Conservative Finite Difference Method for the Heat Equation Jhonnathan Arteaga Arispe, Universidad Simón Bolívar	Adjoint Method for a Tumor Invasion PDE-Constrained Optimization Problem in 2D Using Adaptive Finite Element Method Cristina Turner, Universidad Nacional Córdoba
12:00-14:00	Lunch	

VIII Pan-American WorkShop: Applied and Computational Mathematics

Program - Tuesday, July 22, 2014

14:00-15:00	Invited Presentation	
	Room: Auditorium	
	Christopher Paolini, San Diego State University <u>Thermal-Mechanical Model Coupling in Geologic CO₂ Sequestration Simulation</u> <u>Abstract:</u> An estimated 85% of the world's energy will be derived from fossil fuels by 2030. Mitigating environmental impacts of fossil-fuel combustion on global warming has become a critical issue. With 70% of electricity generated from fossil fuel combustion, CO₂ sequestration in underground aquifer-caprock systems is one solution that is becoming a promising technology for reducing harmful CO₂ emissions created by coal-fired power stations. However, carbon sequestration by injection of CO₂-rich fluids in geologic media is not without risk, as one of the primary fears is the unintentional triggering of small-to moderate-sized earthquakes that can damage the seal integrity of geologic formations that consist of brittle sandstones, which could potentially leak stored CO₂ into the atmosphere. Furthermore, the transport of toxic heavy metals and organic species into fresh water systems can occur through new fractures in caprock formed during CO₂ injection. Stresses resulting from CO₂-rich fluid injection in geologic media may induce rock fracturing. We present a coupled thermal-mechanical model that computes average rockstress,using the Winterfeld-Wu model, as a function of formation temperature, pressure, and hydrologic forces, and is based on the dual porosity model of Aifantis. This average stress model is coupled to a heat-transfer model with a volumetric energy generation source term derived from the revised Helgeson-Kirkham-Flowers (HKF) thermodynamic model for aqueous solute species reactions. The HKF model is based on computing properties of dilute aqueous species by separately considering solvation and nonsolvation contributions. The solvation contribution is based on the Born model for determining the free energy of solvation, where formation water permittivity is calculated using Johnson and Norton regression coefficients. Activity coefficients of electrically charged solutes are approximated using the B-dot model, which is an extended Debye-Hückel model. The HKF derived partial molal heat capacity and enthalpy of charged aqueous species arising from the interaction of CO₂-rich brine with sandstone are used in the source term of a three-dimensional, transient, multiphase heat transfer model. The heat transfer model accounts for the advective and diffusive energy transport of aqueous CO₂,aq, gaseous CO₂,g and natural gas, pure liquid phases (fresh water, oil), and solid rock phases. Advective transport is modeled using Darcy's law for pressure driven-flow and solved using a finite volume method on a staggered grid. Formation pressure is computed using a poroelastic pore pressure diffusion model and solved using the finite element method. Incremental changes in rock permeability are modeled using an Oda permeability tensor that calculates changes in permeability that result from pressure induced fracturing. The impact of rock fractures on fluid flow in a reservoir are determined by the impact fracturing has on permeability, as fractures increase both the magnitude and anisotropy of permeability because of changes in fracture length and hydraulic aperture, properties used to calculate Oda's permeability tensor. Formation porosity and permeability, as a function of rock stress, is determined using the relations of Gutierrez, Rutqvist, and Ostensen. These distinct models for stress, pressure, and temperature are coupled and used to predict fracture characteristics of a shale-sandstone system that models the Oligocene Frio Formation along the Texas Gulf Coast. Simulation results are compared to bottom-hole pressure data obtained from an observation well 30 meters from an injection well during a sequestration test known as the Frio Pilot Experiment.	
	Short Presentations	
	Room: 21G1	Room: 22G1
15:00-15:30	Elliptic Equations with High-Contrast Coefficients and Applications <i>Leonardo Andrés Poveda Cuevas, Universidad Nacional de Colombia</i>	Second- and Fourth-Order Mimetic Discretization of 2-D Elliptic Problems on Equidistributed Grids <i>Jaime Blanco, Universidad Central de Venezuela</i>

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Program - Tuesday, July 22, 2014

	Short Presentations	
	Room: 23G1	Room: 22G1
15:30-16:00	High-Order In-Plane Rupture Simulations on Fully Staggered Grids <i>Adelis Nieves,</i> <i>Universidad Central de Venezuela</i>	Approach for Generating Energy Indicators in Coal Mixtures Gasification for the Analysis of the Synthesis Gas Composition <i>Marlon Bastidas Barranco,</i> <i>Universidad de la Guajira, Colombia</i>
16:00-16:30	Coffee Break	
16:30-18:00	Poster Presentations	
	Room: TBD	
	A New Locally Conservative Lagrangian-Eulerian Method for Hyperbolic Conservation and Balance Laws <i>John Alexander Pérez Sepúlveda,</i> <i>ITM Institución Universitaria</i>	Control Philosophy of a Double Feed Asynchronous Machine for Power Optimization <i>Patricia Sánchez,</i> <i>Universidad Central de Venezuela</i>
	On the Mean Extinction-Time Estimate for Stochastic Population Models <i>Fernando Vadillo,</i> <i>University of the Basque Country</i>	Numerical Simulations of Time-Dependent PDEs <i>Fernando Vadillo,</i> <i>University of the Basque Country</i>
	A Mathematical and Computational Study for Hyperbolic Conservation Laws with Stiff Source Terms <i>Abel Alvarez Bustos,</i> <i>University of Campinas</i>	GUI Development for Pre-Processing Data and its Coupling with a Tsunami Numerical Model <i>Adriana Liendo Sánchez,</i> <i>Venezuelan Foundation for Seismological Research</i>
	Computational Methods for Identification of Clusters in Petrographic Data <i>Camila Martins Saporetti,</i> <i>Federal University of Juiz de Fora</i>	Partial Differential Equations as Three-Dimensional Inverse Moment Problems <i>Maria Beatriz Pintarelli,</i> <i>Universidad Nacional de La Plata</i>

VIII Pan-American WorkShop: Applied and Computational Mathematics

Program - Wednesday, July 23, 2014

07:30-10:30	Registration		
08:30-09:30	Invited Presentation		
	Room: Auditorium		
	Jose M. Cela, Barcelona Supercomputing Center <u>Full Waveform Inversion</u> <u>Abstract:</u> Full waveform inversion (FWI) becomes the new challenge in geophysical exploration. FWI promises an automatic procedure to build useful geophysical models, which improve the quality of the geophysical imaging. Moreover, FWI applied to different kind of waves (elastic---electromagnetic) can be combined to increase the model quality. In order to accomplish those objectives is mandatory to obtain robust FWI algorithms with the required accuracy and scalability on HPC platforms. We present an elastic FWI algorithm for geophysical exploration in oil & gas industry. Our algorithm combines previous developments in elastic forward modeling using mimetic operators and a preconditioner developed for acoustic FWI. This algorithm has been implemented on HPC systems, and it presents a high scalability, with execution times that can be accepted in an industrial environment.		
	Short Presentations		Mini-Workshop
	Room: 23G1		Room: 24G1
09:30-10:00	Analysis of Non Newtonian Blood Flow in Remodeling Radio- Cephalic Fistulas Used in Hemodialysis Process <i>Janaína de Andrade Silva, Federal University of Juiz de Fora</i>		BSIT: An HPC Environment for Exploration Geophysics <i>Jose M. Cela, Barcelona Supercomputing Center</i>
10:00-10:30	Coffee Break		
	Short Presentations		Mini-Workshop
	Room: 21G1	Room: 23G1	Room: 24G1
10:30-11:00	An Upwind Finite Volume Method for the Convection Diffusion Equation on Non-orthogonal Quadrilateral Meshes <i>Giselle Sosa, Universidad Simon Bolivar, Venezuela</i>	Evaluation of a Heart Model Based on Cellular Automata and Mass-Spring Systems <i>Ricardo Silva Campos, Universidade Federal de Juiz e Fora, Brasil</i>	Randomized Linear Algebra in Large Scale Wave Propagation Simulation <i>Victor Pereyra, Stanford University</i>

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Program - Wednesday, July 23, 2014

	Short Presentations		Mini-Workshop
	Room: 21G1	Room: 23G1	Room: 24G1
11:00-11:30	Time-Splitting Scheme for Nonhydrostatic Atmospheric Model <i>Andrei Bourchtein, Pelotas State University, Brazil</i>	Simulation of Coronary Perfusion in the Myocardium Using a Darcy Model for Fluid in Porous Medium <i>João Rafael Alves, Federal University of Juiz de Fora</i>	The Mathematics of Seismic Reflection <i>Miguel Dumett, San Diego State University</i>
11:30-12:00	Modeling Three-Dimensional Winds in Ensenada, Baja California Region <i>Carlos Torres, Mexico National Oceanographic Data Center & Institute for Oceanological Research/UABC</i>	Computational Modeling of Immune Response to Infection by Yellow Fever Virus <i>Carla Rezende Barbosa Bonin, Federal University of Juiz de Fora</i>	Calculating the Probability of Geological Success Prospects: A Critical Review <i>Rober Yibirin, Pacific Rubiales Energy</i>
12:00-14:00	Lunch		
	Short Presentations		Mini-Workshop
	Room: 21G1	Room: 23G1	Room: 22G1
14:00-14:30	Hiperbolicity and Implementation of the WENO Spectral Method with Adaptive Multi-Resolution for the Lighthill-Whitham-Richards Traffic Model <i>Edwin Alberto Bolaño Benitez, Universidad del Norte, Colombia</i>	Simulations of the Anisotropic Electrical Activity of the Heart Using the Lattice Boltzmann Method <i>Joventino Oliveira Campos, Federal University of Juiz de Fora</i>	Reduced-Order Modeling Using Wavelet Transforms <i>Miguel Arguez</i>

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	Short Presentations		Mini-Workshop
	Room: 21G1	Room: 23G1	Room: 22G1
14:30-15:00	Comparative Evaluation of Three Tsunami Models: Goto-Ogawa, GEOCLAW and Delft3D for the 1867 Virgin Islands Scenario and its Effect on the Western Venezuelan Coast <i>Manuel Valera Arriojas, FUNVISIS, Venezuelan Foundation for Seismological Research</i>	On Generation of Spatial Grids for Numerical Models of Geophysical Flows <i>Natalia Naoumova, Pelotas Federal University, Brazil</i>	Uncertainty, Entropy, and Information Value in Exploratory Projects <i>Rober Yibirin, Pacific Rubiales Energy</i>
15:00-15:30	The Simulation of the Hydrodynamics of the Urias Estuary in Mexico <i>Isabel Ramirez, Centro de Investigación Científica y de Educación Superior de Ensenada</i>	Model of the Population Dynamics of Lutzomyia Longiflocosa, Vector of Cutaneous Leishmaniasis in Colombia <i>Gelys Mestre, Universidad de La Salle, Colombia</i>	Structural and Geometric Attributes in Seismic Interpretation <i>German Larrazabal, Jaguar Exploration, Inc.</i>
15:30-16:00	A FEM-Based Study on the Influence of Skewness and Kurtosis Surface Texture Parameters in Human Dental Occlusal Contact <i>Evelyn Aparecida de Oliveira, Federal University of Juiz de Fora</i>	Reverse Engineering of 3D Point Clouds by Means of Curved Triangular Patches <i>Gudrun Albrecht, Université de Valenciennes</i>	FETKIN: Coupling Kinematic Restorations and Temperature to Predict Thrusting, Exhumation Histories, and Thermochronometric Ages <i>Michael Raghib, Ecopetrol - Instituto Colombiano del Petróleo</i>
16:00-16:30	Coffee Break		

VIII Pan-American WorkShop: Applied and Computational Mathematics

Program - Wednesday, July 23, 2014

	Short Presentations		Mini-Workshop
	Room: 21G1	Room: 23G1	Room: 22G1
16:30-17:00	A Singular Value Decomposition-Based Method to Parameterize Three-Dimensional Models Used to Estimate Cardiac Ejection Fraction by Electrical Impedance Tomography <i>Marcos Henrique Fonseca Ribeiro, Federal University of Juiz de Fora, Brazil</i>	Three Dimensional Mimetic Operators on Non Uniform Rectangular Grids <i>Jaime Blanco, Universidad Central de Venezuela</i>	Sparse Regularization for Data Mining and Approximation <i>Reinaldo Sanchez, University of Texas at El Paso</i>
	Short Presentations		
	Room: 21G1	Room: 23G1	
17:00-17:30	Analysis of a Family of Linear Degenerate Parabolic Mixed Equations <i>Ramiro Acevedo, Universidad del Cauca, Colombia</i>	Advances in Multiple Burst-Correcting Codes <i>Ana Lucila Sandoval Orozco, Universidad Complutense de Madrid, Spain</i>	
17:30-18:00	An Adaptive Uzawa Method for the Steady Stokes Equation <i>Catalina Maria Rua Alvarez, Universidad de Nariño</i>	An Efficient Algorithm for Searching Optimal Multiple Burst-Correcting Codes <i>Ana Lucila Sandoval Orozco, Universidad Complutense de Madrid, Spain</i>	

VIII Pan-American WorkShop: Applied and Computational Mathematics

Program - Thursday, July 24, 2014

07:30-10:30	Registration	
08:30-09:30	Invited Presentation	
	Room: Auditorium	
	Godela Scherer, University of Reading, UK & Universidad Simón Bolívar, Venezuela <u>Moving Mesh Finite Difference Schemes for Nonlinear Time-Dependent PDE</u> <u>Abstract:</u> This is a review of some recently designed velocity-based moving mesh (MM) numerical methods. We are interested in schemes that, with an available fixed number of nodes, are able to adjust to the evolution of the solution and track moving boundaries and other singular solution behaviour like large solution variations. We consider PDE problems that are scale-invariant and mass conserving and describe several MM finite difference schemes based on a conservation principle to control the mesh evolution. Two coupled equations need to be solved, the PDE and an equation for the mesh and we analyse some implicit and semi-implicit time-stepping schemes for the latter. Since these MM methods aim to preserve either local or distributed properties in time it is important to represent the initial data in the best possible way in the L_2-norm. We compare several algorithms in 1 and 2D that choose an initial mesh with an optimal node distribution for the given initial conditions.	
	Short Presentations	
	Room: 21G1	
09:30-10:00	Mimetic and Standard Finite Difference Approaches to Modeling the Diffusion of Calcium Within a Single Sarcomere of an Adult Cardiomyocyte <i>Rosa Lemus, San Diego State University</i>	
10:00-10:30	Coffee Break	
	Short Presentations	
	Room: 22G1	Room: 21G1
10:30-11:00	Variational Methods for Meshless Approximation of Surfaces: Comparing the FEM <i>Alberto Hananel Baigorria, Universidad de Granada/Universidad Católica Santo Toribio de Mogrovejo</i>	Mimetic Methods for Welding Plates Problems <i>Giselle Sosa, Universidad Simon Bolivar, Venezuela</i>

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Program - Thursday, July 24, 2014

	Short Presentations	
	Room: 22G1	Room: 21G1
11:00-11:30	A Least Squares Warping Algorithm for PP/PS Reflectors Matching in Pre-Stack Depth Migrated Images <i>Miguel Dumett,</i> <i>San Diego State University</i>	A Parallel 3D Numerical Simulation of Hyperthermia Cancer Treatment Considering a Nonlinear Bioheat Transfer Model <i>Ruy Freitas Reis,</i> <i>Universidade Federal de Juiz de Fora</i>
	Room: 22G1	
11:30-12:00	Compact Finite Difference Modeling of 2-D Acoustic Wave Propagation <i>Luis Cordova,</i> <i>Universidad de Oriente, Venezuela</i>	
12:00-14:00	Lunch	
	Short Presentations	
	Room: 22G1	Room: 25G1
14:00-14:30	Numerical Analysis of the Acoustics of a Diffusion Flame <i>Charles Quevedo Carpes,</i> <i>Universidade Federal do Pampa</i>	Estimation of Error and Adaptativity in Mimetic Methods <i>Giovanni Calderón,</i> <i>Universidad de Los Andes</i>
	Room: 25G1	
14:30-15:00	Data Assimilation for an Operational System in the Bay of San Quintin <i>Mariangel Garcia,</i> <i>San Diego State University</i>	
	Room: 22G1	Room: 25G1
15:00-15:30	Numerical Analysis of Methane Combustion in Porous Media <i>Elisângela Pinto Francisquetti,</i> <i>Federal University of Rio Grande do Sul</i>	K-Exponential Statistical Manifold Modeled on Orlicz Spaces <i>Héctor Román Quiceno Echavarría,</i> <i>Instituto Tecnológico Metropolitano</i>

VIII Pan-American WorkShop: Applied and Computational Mathematics

Program - Thursday, July 24, 2014

	Short Presentations	
	Room: 22G1	Room: 25G1
15:30-16:00	Analysis of a Model Developed for Reactive Flow in Porous Media <i>Elisângela Pinto Francisquetti, Federal University of Rio Grande do Sul</i>	Using Weak Forms to Derive Asymptotic Expansions of Elliptic Equations with High-Contrast Coefficients <i>Sebastian Huepo Beltran, Universidad Nacional de Colombia</i>
16:00-16:30	Coffee Break	
	Short Presentations	
	Room: 22G1	
16:30-17:00	Temperature and Water Age Simulation of a Reservoir in Central Mexico <i>Eric Gutierrez, National Water Commission, México</i>	

VIII Pan-American WorkShop: Applied and Computational Mathematics

Program - Friday, July 25, 2014

08:30-09:30	Invited Presentation
	Room: Auditorium
	Lothar Banz, Leibniz Universität Hannover <u>hp -Adaptive FEM for Elliptic Ocstacle Problems CG vs. IPDG</u> <u>Abstract:</u> The solution of an elliptic obstacle problem is typically only of reduced regularity, with a singularity across the a priori unknown free boundary. It is therefore apparent that <i>hp</i>-adaptive FEM is an appropriate tool for solving that problem approximately. Here, the non-penetration condition is enforced weakly by a Lagrange multiplier λ leading to a mixed method. On the discrete level the Lagrange multiplier λ_{hp} is a linear combination of basis functions which are biorthogonal to the basis functions of the primal variable. This allows to use the same mesh and polynomial degree for both the primal and dual variable. For both the continuous Galerkin (cG) and the interior penalty discontinuous Galerkin (IPDG) method a residual based a posteriori error estimator is derived. These consist of a discretization error of a linear variational equality problem, a consistency term in λ_{hp}, a complementarity term and an obstacle penetration term. For the IPDG an additional consistency term in $\mathcal{U}_{hp}$ arises. In the second part of the talk we describe how the connectivity matrices for biorthogonal basis functions can be computed efficiently, even in the presence of multiple order hanging nodes and anisotropic meshes. In the numerical experiments we compare cG with IPDG and show the applicability of the derived error estimations and the superiority of <i>hp</i>-adaptivity compared to low order uniform and adaptive approaches. The results on cG, IPDG are based on joint work with Andreas Schröder, Ernst P. Stephan, respectively.
9:30-10:30	Awards Presentation
10:30-18:00	Excursion to Barranquilla

Invited Presentations

Monday, July 21, 2014 - 9:30am-10:30am, Auditorium

Mimetic Discretization Methods

By Jose Castillo

San Diego State University

Mimetic compatible discretizations have been a recurrent theme in the history of numerical methods for solving partial differential equations with variable degree of success. There are many investigations currently active in this area, pursuing different approaches and many algorithms have been developed along these lines. Loosely speaking, “mimetic” or “compatible” algebraic methods have discrete structures that mimic vector calculus identities and theorems. Specific approaches to discretization have achieved this compatibility following different paths, and with diverse degree of generality in relation to the problems solved and the order of accuracy obtainable. Here, we present theoretical aspects of a mimetic method based on the extended Gauss Divergence Theorem as well as examples by means of the Mimetic methods to solve partial differential equations using the Mimetic Library Toolkit (MTK).

Monday, July 21, 2014 - 2:00pm-3:00pm, Auditorium

hp-Adaptive BEM For Frictional Contact Problems In Linear Elasticity

By Ernst Stephan

Leibniz Universität Hannover

A mixed formulation for a Tresca frictional contact problem in linear elasticity is considered in the context of boundary integral equations, which is later extended to Coulomb friction. The discrete Lagrange multiplier, an approximation of the surface traction on the contact boundary part, is a linear combination of biorthogonal basis functions. In case of curved elements, these are the solutions of local problems. In particular, the biorthogonality allows to rewrite the variational inequality constraints as a simple set of complementarity problems. Thus, enabling an efficient application of a semi-smooth Newton solver for the discrete mixed problem, converging locally super-linearly in the frictional case and quadratically in the frictionless case. Typically, the solution of frictional contact problems is of reduced regularity at the interface between contact to non-contact and from stick to slip. To identify the a priori unknown locations of these interfaces two a posteriori error estimations are introduced. In a first step the error is split into specific error contributions resulting from the contact and friction conditions and from the discretization error of a variational equation. For the latter a residual and a bubble error estimation are considered explicitly. The numerical experiments show the applicability of the derived error estimations, in particular in the Coulomb friction case, and the superiority of hp-adaptivity compared to low order uniform and adaptive approaches.

Tuesday, July 22, 2014 - 8:30am-9:30am, Auditorium

Seismic Survey Simulation and Imaging in 3D

By Victor Pereyra

Stanford University

Current distributed computing systems allow the simulation of very large seismic surveys consisting of thousands of source-receiver pairs by using the full wave equation. Imaging, such as Reverse Time Migration, also has similar requirements. The clock time required, though, is still fairly significant and it is of interest to see if it can be reduced. In previous work we have shown that Model Order Reduction applied to the 2D acoustic wave equation could produce speed-ups of one order of magnitude when applied to these problems. In principle, there are no conceptual difficulties in extending these techniques to 3D. However, the requirements for existing applications make it more challenging due to the large size simulations involved and the fact that one is restricted to work in a single multicore box for each source-receiver pair. Even with upper end machines, there are difficulties and we will discuss in this talk some proposed alternatives to existing algorithms.

Tuesday, July 22, 2014 - 2:00pm-3:00pm, Auditorium

Thermal-Mechanical Model Coupling in Geologic CO₂ Sequestration Simulation

By Christopher Paolini

San Diego State University

An estimated 85% of the world's energy will be derived from fossil fuels by 2030. Mitigating environmental impacts of fossil-fuel combustion on global warming has become a critical issue. With 70% of electricity generated from fossil fuel combustion, CO₂ sequestration in underground aquifer-caprock systems is one solution that is becoming a promising technology for reducing harmful CO₂ emissions created by coal-fired power stations. However, carbon sequestration by injection of CO₂-rich fluids in geologic media is not without risk, as one of the primary fears is the unintentional triggering of small-to moderate-sized earthquakes that can damage the seal integrity of geologic formations that consist of brittle sandstones, which could potentially leak stored CO₂ into the atmosphere. Furthermore, the transport of toxic heavy metals and organic species into fresh water systems can occur through new fractures in caprock formed during CO₂ injection. Stresses resulting from CO₂-rich fluid injection in geologic media may induce rock fracturing. We present a coupled thermal-mechanical model that computes average rock stress, using the Winterfeld-Wu model, as a function of formation temperature, pressure, and hydrologic forces, and is based on the dual porosity model of Aifantis. This average stress model is coupled to a heat-transfer model with a volumetric energy generation source term derived from the revised Helgeson-Kirkham-Flowers (HKF) thermodynamic model for aqueous solute species reactions. The HKF model is based on computing properties of dilute aqueous species by separately considering solvation and nonsolvation contributions.

The solvation contribution is based on the Born model for determining the free energy of solvation, where formation water permittivity is calculated using Johnson and Norton regression coefficients. Activity coefficients of electrically charged solutes are approximated using the B-dot model, which is an extended Debye-Hückel model. The HKF derived partial molal heat capacity and enthalpy of charged aqueous species arising from the interaction of CO₂-rich brine with sandstone are used in the source term of a three-dimensional, transient, multiphase heat transfer model. The heat transfer model accounts for the advective and diffusive energy transport of aqueous CO₂,aq, gaseous CO₂,g and natural gas, pure liquid phases (fresh water, oil), and solid rock phases. Advective transport is modeled using Darcy's law for pressure driven-flow and solved using a finite volume method on a staggered grid. Formation pressure is computed using a poroelastic pore pressure diffusion model and solved using the finite element method. Incremental changes in rock permeability are modeled using an Oda permeability tensor that calculates changes in permeability that result from pressure induced fracturing. The impact of rock fractures on fluid flow in a reservoir are determined by the impact fracturing has on permeability, as fractures increase both the magnitude and anisotropy of permeability because of changes in fracture length and hydraulic aperture, properties used to calculate Oda's permeability tensor. Formation porosity and permeability, as a function of rock stress, is determined using the relations of Gutierrez, Rutqvist, and Ostensen. These distinct models for stress, pressure, and temperature are coupled and used to predict fracture characteristics of a shale-sandstone system that models the Oligocene Frio Formation along the Texas Gulf Coast. Simulation results are compared to bottom-hole pressure data obtained from an observation well 30 meters from an injection well during a sequestration test known as the Frio Pilot Experiment.

**Wednesday, July 23, 2014 - 8:30am-9:30am,
Auditorium**

Full Waveform Inversion

By Jose M. Cela

Barcelona Supercomputing Center

Full waveform inversion (FWI) becomes the new challenge in geophysical exploration. FWI promises an automatic procedure to build useful geophysical models, which improve the quality of the geophysical imaging. Moreover, FWI applied to different kind of waves (elastic--electromagnetic) can be combined to increase the model quality. In order to accomplish those objectives is mandatory to obtain robust FWI algorithms with the required accuracy and scalability on HPC platforms. We present an elastic FWI algorithm for geophysical exploration in oil & gas industry. Our algorithm combines previous developments in elastic forward modeling using mimetic operators and a preconditioner developed for acoustic FWI. This algorithm has been implemented on HPC systems, and it presents a high scalability, with execution times that can be accepted in an industrial environment.

Thursday, July 24, 2014 - 8:30am-9:30am, Auditorium
Moving Mesh Finite Difference Schemes for Nonlinear Time-Dependent PDE

By Godela Scherer

University of Reading, UK & Universidad Simón Bolívar, Venezuela

This is a review of some recently designed velocity-based moving mesh (MM) numerical methods. We are interested in schemes that, with an available fixed number of nodes, are able to adjust to the evolution of the solution and track moving boundaries and other singular solution behaviour like large solution variations. We consider PDE problems that are scale-invariant and mass conserving and describe several MM finite difference schemes based on a conservation principle to control the mesh evolution. Two coupled equations need to be solved, the PDE and an equation for the mesh and we analyse some implicit and semi-implicit time-stepping schemes for the latter. Since these MM methods aim to preserve either local or distributed properties in time it is important to represent the initial data in the best possible way in the L_2 -norm. We compare several algorithms in 1 and 2D that choose an initial mesh with an optimal node distribution for the given initial conditions.

Friday, July 25, 2014 - 8:30am-9:30am, Auditorium
hp-Adaptive FEM for Elliptic Obstacle Problems CG vs. IPDG

By Lothar Banz

Leibniz Universität Hannover

The solution of an elliptic obstacle problem is typically only of reduced regularity, with a singularity across the a priori unknown free boundary. It is therefore apparent that hp-adaptive FEM is an appropriate tool for solving that problem approximately. Here, the non-penetration condition is enforced weakly by a Lagrange multiplier λ leading to a mixed method. On the discrete level the Lagrange multiplier λ_{hp} is a linear combination of basis functions which are biorthogonal to the basis functions of the primal variable. This allows to use the same mesh and polynomial degree for both the primal and dual variable. For both the continuous Galerkin (cG) and the interior penalty discontinuous Galerkin (IPDG) method a residual based a posteriori error estimator is derived. These consist of a discretization error of a linear variational equality problem, a consistency term in λ_{hp} , a complementarity term and an obstacle penetration term. For the IPDG an additional consistency term in U_{hp} arises. In the second part of the talk we describe how the connectivity matrices for biorthogonal basis functions can be computed efficiently, even in the presence of multiple order hanging nodes and anisotropic meshes. In the numerical experiments we compare cG with IPDG and show the applicability of the derived error estimations and the superiority of hp-adaptivity compared to low order uniform and adaptive approaches. The results on cG, IPDG are based on joint work with Andreas Schröder, Ernst P. Stephan, respectively.

Monday, July 21, 2014 - 10:30am-11:00am, 22G1

Second-Order Mimetic Discretization of the Seismic Wave Equation in Heterogeneous Media

By Freysimar Solano Feo

Universidad Central de Venezuela

The cornerstone of mimetic finite differentiation (FD) is that discrete gradients and divergences, in combination to a novel boundary flux operator satisfy an approximation to the Gauss Divergence theorem. In this paper, we propose a spatially staggered second-order discretization of the acoustic wave equation that fully exploits all these mimetic operators in the implementation of free surface and absorbing boundary conditions. Explicit time integration is carried out by using the standard three-level central FD stencil. We present a stability and convergence analysis of this new scheme and use a traditional nodal second-order FD method as reference. A family of numerical tests with a common free-surface boundary layer is used to show the higher accuracy and similar experimental convergence of the mimetic method relative to the nodal FD scheme. Applications of this new method to simple 2-D seismic scenarios are also presented and discussed.

Monday, July 21, 2014 - 10:30am-11:00am, 23G1

Mathematical Modeling of a Direct Bioethanol Pem Fuel Cell

By R.S. Gomes

Federal University of Rio Grande do Sul

The energy consumption has grown over the years, and the combustion process is mainly responsible to transform energy. However, the environmental awareness and the increasing prices of fossil fuels have motivated many experts to look for renewable energy sources. Furthermore, easy access to fossil fuel resources are limited and are expected to end in the forthcoming future.

Fuel cells are devices where the electrochemical oxidation of a fuel occurs. Fuel cells present higher efficiency and safety when compared with internal combustion engines. Furthermore, they are a good alternative for energy generation because, in addition to being efficient and reliable, they generate low pollution and can use several types of fuels. The bioethanol is a fuel produced generally by fermentation of sugar of plants. It is produced from many agricultural products and food waste that contains cellulose, sugar or starch.

For the numerical implementation and development of a direct bioethanol fuel cell is necessary to understand the kinetic mechanisms. Detailed kinetic mechanisms for the bioethanol oxidation involve a large number of species in different timescales, which induces stiffness in the governing equations. Therefore, it is necessary to use a reduced mechanism for the bioethanol,

here with seven reactions, which preserves accuracy and fidelity of the detailed mechanism with much less computational effort.

High-performance computing and advanced numerical algorithms have allowed researchers to model proton exchange membrane (PEM) fuel cells. The structure of a simple PEM includes an anode, an electrolyte, and a cathode. PEM fuel cell operations involve simultaneously multi-component, multi-phase, multi-dimensional fluid flow with heat transfer and mass transfer and electrochemical reactions. Therefore, a mathematical model is necessary to characterize the fuel cells physical behavior.

In this work we have developed a mathematical model to analyze a direct bioethanol PEM fuel cell consisting of the following equations: mass conservation, momentum conservation, volume fraction, energy conservation, species transport and conservation of charge. The numerical simulation of the reactive flow was developed based on the central finite difference method. The equations were integrated in the time using the simplified Runge-Kutta multistage scheme. Obtained results are in agreement with data found in the literature. Since there is not a general model to analyze fuel cells, this paper contributes to understand available models and their numerical simulation.

Monday, July 21, 2014 - 11:00am-11:30am, 22G1

Performance Analysis of a Mimetic Finite Difference Scheme for Acoustic Problems: CPU Versus GPU Computing

By Otilio Rojas

Universidad Central de Venezuela

Nowadays, numerical simulations of seismic propagation phenomena demand high performance computing because of the large study domain of interest and the high volume of input/output data. In the case of finite difference methods (or any other volume discretization scheme), processing time might become strikingly large if we additionally use well refined grids in order to capture small physical devices on wave patterns.

In this paper, we present several C implementations of a mimetic finite difference method for acoustic wave propagation on highly dense staggered grids. These implementations evolve as different optimization strategies are implemented starting from code vectorization by using SSE and AVX instructions, appropriate setting of compilation flags, CPU parallelization by exploiting the OpenMP framework, to the final code parallelization on GPU platforms. We present and discuss the increasing computation speed up of this mimetic scheme achieved by the gradual implementation and testing of all these performance optimizations.

Monday, July 21, 2014 - 11:00am-11:30am, 23G1

Development of Reduced Kinetic Mechanisms for Propane and N-Heptane Diffusion Flames

By R.S. Gomes

Federal University of Rio Grande do Sul

Propane is one of the simplest hydrocarbons that can be a representative of higher hydrocarbons used in many applications. Propane is rapidly consumed on the rich side of the flames to produce a large amount of C1 and C2 intermediates, principally at low strain rate conditions. This behavior is similar to the combustion of hydrocarbon fuels more complex. From a mathematical point of view, a mechanism for the combustion of propane, compared to other higher hydrocarbons, requires a smaller number of species and reactions for a detailed study of the kinetics of chemical reactions.

The n-heptane is a high chain hydrocarbon fuel, which is adapted as a surrogate for some liquid fuels used in many propulsion and power generation systems. The n-heptane cetane number is approximately 56, which is typical for diesel fuel, as its ignition and combustion properties are similar to those of diesel fuel. The n-heptane has received substantial interest because it is a major component of the primary reference fuel (PRF) in internal combustion engine studies.

The numerical simulations of detailed kinetic mechanisms for large hydrocarbons are complicated by the existence of highly reactive radicals which induces significant stiffness to the equations, due to the big differences in the time scales of the species. Consequently, there exists the need to develop, from these detailed mechanisms, the corresponding reduced mechanisms of fewer variables and moderated stiffness, while maintaining the accuracy and comprehensiveness of the detailed mechanism.

Detailed kinetic mechanisms describing hydrocarbon combustion seems to be structured in a hierarchical manner. The principal path for the H₂ belongs to the chain for the CO, that is part of the chain for the ethylene, which belongs to the principal paths for the propane and the n-heptane. Since it is difficult to write manually such mechanisms, they are generated by an automated procedure for convenience.

Based on a kinetic mechanism composed by 82 reactions among 30 species, it is developed a seven-step mechanism among 14 species for the propane. A chemical mechanism composed by about 1500 reactions among 160 species is reduced to obtain a thirteen-step kinetic mechanism among 16 species for the n-heptane. The reduction strategy consists in applying the sensitivity analysis to obtain the skeletal mechanism, estimating the order of magnitude of reaction rates, defining the main chain, applying the hypotheses of steady-state and partial equilibrium and in justifying the assumptions through an asymptotic analysis. The asymptotic analysis employs the concept of limits

to identify reactions, critical conditions and other important parameters. In this analysis, the steady-state assumption for a species leads to algebraic equations among reaction rates.

Numerical tests were carried out to validate the mechanisms. The discretization followed the central finite difference scheme based on the Runge-Kutta multistage integrator. Obtained results compare favorably with data found in the literature for both propane and n-heptane jet diffusion flames.

It is frequently found different reduced kinetic mechanisms for the same fuel in the literature. Since it seems that there is not an universal method to generate such mechanisms, the principal contribution of this paper is the development of consistent mechanisms for propane and n-heptane, as well as, their validation through sensitive and asymptotic analysis.

Monday, July 21, 2014 - 11:30am-12:00pm, 22G1

Mimetic Discretization of Fourth-Order Hyperbolic Equations on Spatial-Time Staggered Grids

By Freysimar Solano Feo

Universidad Central de Venezuela

We present a novel mimetic finite difference (FD) scheme for modeling elastic motion of a thin beam with general end conditions. Governing mathematical model comprises a fourth-order hyperbolic equation to describe displacement of interior beam points and general Robin boundary conditions. We discretize this model on a staggered grid in both space and time domains, combining second-order spatial mimetic operators and central time differentiation of the equivalent system for beam particle velocity and displacement laplacian. In this paper, we present a formal stability analysis of this mimetic scheme and numerically explore its convergence properties. Relative to a standard FD method designed on nodal grids, the mimetic scheme exhibits higher precision and faster convergence on numerical tests reported in this work.

Monday, July 21, 2014 - 11:30am-12:00pm, 23G1

Modeling Supershear Rupture Propagation on Rate and State Faults Accounting for Thermal Pressurization of Pore Fluids

By Adelis Nieves

Universidad Central de Venezuela

On the process of earthquake ruptures two main mechanisms that weaken fault strength are the fast rupturing of microscopic asperity contacts at seismic sliding velocities known as Flash Heating (FH), and the reduction of the compressive tectonic load by the Thermal Pressurization (TP) of pore fluids. Earthquakes and also experimentally reproduced spontaneous ruptures may propagate as slip pulses (sliding is highly localized on the pulse region) or cracks (slip continues growing everywhere within the rupture zone). On the other hand, rupture speed is usually

sub-Rayleigh but there are emergent geological, experimental, and numerical studies that support propagation transitioning to supershear velocities. Propagation on alternative rupture modes (pulses vs cracks) is attributed to the background shear loading (Zheng and Rice; 1998), while sub-Rayleigh-to-Supershear speed transition is also explained in terms of loading conditions and the frictional fault behavior (Andrew; 1976,1985). In this work, we conduct simulations of mode II ruptures along a planar fault obeying a rate- and state-dependent friction law (RS) and use the Mimetic Operators with Split Nodes (MOSN) finite difference method. MOSN presents consistent fourth-order spatial accuracy in the whole fault-elastic domain combined to implicit ODE integration in time (either Euler or Trapezoidal) to evolve the velocity-state fault system given its high initial stiffness. Here, we incorporate a semi-analytical integration of the coupled TP diffusion equations for temperature and pore pressure evolution into MOSN by means of efficient memory variables. Finally, we use this new MOSN method to study the dependency of rupture mode generation and propagation velocity on the initial and constitutive parameters of this RS-FH-TP fault model.

Monday, July 21, 2014 - 3:00pm-3:30pm, 23G1

Optimally Accurate Mimetic Finite Difference Modeling of Free Surfaces on Elastic Media

By Luis Cordova

Universidad de Oriente, Venezuela

High-order Castillo-Grone mimetic gradient and divergence approximations represent a multi-parametric family of conservative finite differences that preserve an integration by parts formula in discrete form. The number of free parameters on such mimetic operators is tied to the construction accuracy and their setting on current applications only aims to reduce stencil lengths on the grid neighborhood of boundary points. In this work, we assess the influence of mimetic parameters on the dispersion errors of fourth-order numerical simulations of elastic waves on 1-D and 2-D domains. Dispersion curves of our mimetic solvers are obtained by both a standard 1-D theoretical analysis and the estimation of the phase difference of traveling Rayleigh pulses along the free surface of a 2-D half plane. Stable and low dispersive mimetic parameters are finally proposed for optimal fourth-order simulation of elastic motion.

Monday, July 21, 2014 - 3:00pm-3:30pm, 24G1

Analysis of Double Feed Asynchronous Machine in Eolic Generation

By Patricia Sánchez

Universidad Central de Venezuela

In Eolic generation, double feed asynchronous is highly used because it allows obtaining stable parameters through the control of rotative currents vector. Therefore, it is necessary to

maintain a trustworthy control. The objective of this research is to identify the dynamic behavior of the turbine-asynchronous machine system, considering the reactive power delivered to the grid, in such a manner, that it can cover its requirements in real time. The operation of the double feed asynchronous machine was studied and the simulation of the system was carried out to test its behavior. We found that this configuration allows controlling all the output parameters: power factor, torque, frequency and phase, which allows the optimization of the wind turbine. We also found that if the torque generated by the wind turbine is combined with the torque produced in the asynchronous machine, the maximum efficiency point can be continuously tracked.

Monday, July 21, 2014 - 3:30pm-4:00pm, 23G1

Discrete Mollification and the Numerical Solution of Problems Associated to Partial Differential Equations
By Carlos E. Mejía

Universidad Nacional de Colombia

Discrete mollification is a convolution-based filtering procedure for the regularization of ill-posed problems and the stabilization of explicit schemes for the numerical solution of partial differential equations. In this talk we review the benefits that discrete mollification brings to a variety of finite difference explicit schemes. In a first group, the gain is in acceleration of computations through an improvement of the CFL condition. The second group consists of problems in which the numerical estimation of parameters is sought and it includes our more recent work. For the problems of this group, discrete mollification enhances stability and allows effective parameter identification procedures. To illustrate the numerical performance of the algorithms, several numerical examples are presented.

Monday, July 21, 2014 - 3:30pm-4:00pm, 24G1

Numerical Simulation of a Tool to Detect Vulnerable Areas in Case of Tsunamis: A Web Map Service Implementation for Venezuelan Coasts

By Miguel Rojas

Venezuelan Foundation for Seismological Research

The geographic portal allows entry of any geolocation data by users (latitude and longitude), thus it is possible to find the most probable tsunamigenic scenario, based on the minimum epicentral distance. Both, historical records of tsunamis that have affected the Venezuelan coast and data input of the previously calculated results of the numerical model in the database are used. Documents such as maximum heights, flood charts and Tsunami arrival time are introduced into the geographic portal. Geographic Information Systems (GIS) that overlay analysis and defined security zones and optimized evacuation routes data are used too. This information is accessible through the developed geographic portal using open source. This tool will provide under the standards of the Open Geospatial Consortium

(OGC) free access to information. All scenarios in the Web Map Service (WMS) layers overlap with Google map and Google earth repositories, so all information can be displayed for warning of possible occurrence of a tsunami. The most important contribution of this work is to enable decision makers to have tools that allow, by a quickly and easy way, to find the possible areas to be affected when a tsunami occurs, so in this way they can cooperate with institutes for prevention and mitigation of disasters in an effective evacuation to protect the population.

Monday, July 21, 2014 - 4:30pm-5:00pm, 23G1

Applying Mimetic Finite Differences and Model Order Reduction to 2-D Seismic Wave Propagation

By Otilio Rojas

Universidad Central de Venezuela

Despite the progress on computing technology, some applications on hydrocarbon exploration involving simulations of seismic motion on realistic large scale domains are still too costly for most current CPU clusters. For instance, high fidelity forward simulations of wave propagation induced by multiple shoots represent a computationally intensive step on standard seismic migration and inversion platforms when using a volume discretization numerical method. In this work, we exploit a Model Order Reduction (MOR) strategy by the proper orthogonal decomposition (POD) of few full wave simulations and extract the fundamental dynamical modes of wave phenomena. Subsequent wave interactions on either original simulations or alternative tests for different parameter sets, are a posteriori estimated by the time integration of a reduced dynamical system constructed from the POD output modes. To feed this MOR framework, we employ a new high-order mimetic scheme on spatially staggered grids to compute the POD preceding full wave finite difference simulations. Accuracy and computation speed-up of our MOR scheme is assessed using full FD mimetic simulations along the whole simulation time as reference.

Monday, July 21, 2014 - 4:30pm-5:00pm, 24G1

Short-Term Load Forecasting Using an Updated Load Curve Formulation

By Guilherme Guilhermino Neto

Universidade Federal de Juiz de Fora

Electrical load forecasting, for a wide range of lead times, is a vital task in the managing of power systems. In order to build the production plan, which includes generation and dispatching schedules, an utility must estimate its short-term demand (usually for the entire next day). Since it is not possible to keep large energy inventories for meeting sudden load increases and, on the other hand, overproduction could lead to physical and financial damages, it is extremely important to have accurate and reliable forecasts. Several techniques have been proposed

to solve the load forecasting problem. Some of them make forecasts based on the series of past loads, due to the seasonal behaviour of the electricity demand, but some take into account the fact that weather variables (as temperature, humidity or wind speed) may cause deviations from the average load. Recent, neural networks, fuzzy logic and other computational intelligence techniques have been very popular as tools for load forecasting, using information from past loads and weather. These methods can lead to forecasts with very low errors; however, because of their extreme nonlinearity, they may also lead sometimes to outliers, or to hard-to-interpret results. This paper proposes a model inspired on the load curve formulations which were popular in the 1980s and 1990s, but updated by the inclusion of some recently developed techniques. In this model, the demand is written as a linear combination of a 'base load' (modeled as a linear function of the past loads), with a 'weather-related load' (modeled as a function of the temperature of the air). The Holt-Winters-Taylor exponential smoothing method is used to estimate the base load, and either a regression model or a neural network is used to estimate the contribution of the weather. In this way, we manage to combine the robustness of the linear methods, with the flexibility of the nonlinear ones. This combination model is tested on two data sets, and is shown to outperform various other statistical and computational benchmarks.

Monday, July 21, 2014 - 5:00pm-5:30pm, 23G1

Effect of Wind Direction and Orography on Flow Structures at Baja California Coast: A Numerical Approach

By Carlos R. Torres

Mexico National Oceanographic Data Center & Institute for Oceanological Research/UABC

In order to study the effect of orography and wind direction on flow structures of the Baja California Coast, the momentum primitive equations describing an atmospheric flow over that region were solved numerically employing the General Curvilinear Atmospheric Model (Torres et al. 2014). Simulations were performed for varying wind direction and compared to available observations. Wind stress and other variables of interest were also calculated.

Monday, July 21, 2014 - 5:00pm-5:30pm, 24G1

On Fractal Dimensions of Natural and Artificial Environments

By Natalia Naoumova

Pelotas Federal University, Brazil

Application of the fractal theory to the study of the complexity of natural and built environments has a short history, but it is shown to be useful both for the investigation of the relations between constructed sites and surrounding geographic

places and for the definition of the optimal design of planned constructions. In this study, we employ the optimized box-counting algorithm to analyze the level of visual complexity of two historical Brazilian sites. Different parameters of a general box-counting method, including the choice of space scales, grid location and box ratio coefficient, are evaluated in order to determine a stable and reliable version of the method. The optimized algorithm is applied for evaluation of the visual complexity of two different (mountain and coastal) landscapes and the corresponding historical sites. The obtained results provide the evidence that there exists a strong connection between the levels of fractal complexity of the historical parts of the cities and their geographical environments.

Monday, July 21, 2014 - 5:30pm-6:00pm, 23G1
Building Orthogonal Grids Using Lemniscates
By Gustavo Adolfo Restrepo
Universidad Nacional de Colombia

We consider the problem of building orthogonal grids on meandering like regions; these are similar to riverbeds and to longitudinal sections of tubular objects. High quality grids on such region are necessary for the numerical treatment of PDE's.

The special geometry of meandering like regions allows for the use of conformal techniques to build the grid. Cardona-Lentini-Paluszny [2010] and Lentini-Paluszny [2013] used lemniscates for orthogonal meshing of such regions. Their process consisted in building a sequence of lemniscatic sectors that fit the region: the construction of a lemniscate sectors (i.e. a region between two confocal lemniscates and two orthogonal rays) depends on the previous sector and each step requires an optimization procedure.

We propose a non-sequential alternative, for which we consider a reference database of lemniscatic sectors augmented with a set of regions bounded by ellipses and hyperbolas, and compare not too long arbitrary sectors of the meandering like region with elements of the database.

Tuesday, July 22, 2014 - 9:30am-10:00am, 21G1
On Perturbations of Principal Eigenvalues of Substochastic Matrices
By Andrei Bourchtein
Pelotas State University, Brazil

In this report, we consider the row-substochastic matrices with some zero rows and analyze how their principal eigenvectors, that is the eigenvectors corresponding to the spectral radius of the matrix, are changed under substitution of zero rows by a row-stochastic vector. Possible applications to computation of the PageRank vector, used by Google to rank web pages, are considered. In particular, the considered modifications of

row-substochastic matrices correspond to substitution of the dangling nodes by artificial links in the original web matrix. By this analogy, our analysis can be used to clarify when the choice of the dangling vector does not change the eigenvectors of the original web matrix and to provide evaluations for perturbations of the principal eigenvectors when they are modified.

Tuesday, July 22, 2014 - 9:30am-10:00am, 22G1
A Fuzzy Optimization Model for Berth Allocation Problem to Vessels Arriving with Delay
By Flabio Gutierrez
Universidad Nacional del Peru

The berth allocation problem (BAP) in a maritime container terminal is defined as a feasible allocation of berths to incoming vessels. In this paper, we developed a fuzzy mathematical programming model for continuous and dynamic BAP. It is assumed that the arriving time of vessels is imprecise, in the sense that the vessels can have a delay but only up to a permitted tolerance. Fuzzy sets are used to represent the imprecision. The proposed model has been codified in CPLEX solver and evaluated in different instances. The obtained results shows that the proposed model can help the container terminal managers, since it has available berth plans with different degrees of allowed delay, which are optimized according to the waiting time. One of the model's features is that, as a vessel has more possibilities to be late, the model grants her a fuzzy berth time that supports that delay.

Tuesday, July 22, 2014 - 10:30am-11:00am, 21G1
On Improving The Block Variable Conjugate Gradient Algorithm
By Pedro Torres
National University of Asuncion

In this work we present a new strategy for varying the block size of the Block Conjugate Gradient, for solving a linear system with a single right hand side. We explore and compare this with other existing strategies. Measurement of performance for each approach is given, using the relatively recent improvement of the kernel Sparse Matrix-Matrix (SpMM) multiplications. The results with this strategy are promising, if we implement this using multivector optimizations.

Tuesday, July 22, 2014 - 10:30am-11:00am, 22G1
Comparison of Techniques of Adaptive Penalty on Artificial Bee Colony Algorithm Applied to Optimization Problems in Engineering
By Grasielle Regina Duarte
Universidade Federal de Juiz e Fora, Brasil

Nature-inspired algorithms have been proposed for solving complex search and optimization problems in various areas of Science and Engineering. Some examples of such algorithms are Genetic Algorithms, Particle Swarm Optimization, Ant Colony Optimization, and Artificial Bee Colony Algorithm (ABC).

The ABC, inspired by the foraging behavior of real bees in colonies, is an algorithm recently proposed for the solution of numerical optimization problems. In this algorithm, three types of bees are involved in the search process:

- (1) the employed bees that leave the colony in search of food and through dance, share information about the source with other bees;
- (2) the onlooker bees that select sources they deem advantageous according to information received and
- (3) the scout bees that leave the colony performing a random search for new food sources.

In ABC, the food sources represent possible solutions to the problem, and every food source has an employed bee associated with it.

Food sources that do not have their quality improved in a number of cycles are replaced by new random positions, which are determined by scout bees.

The ABC was originally proposed for solving unconstrained optimization problems. The algorithm has been shown to be competitive with other meta-heuristics and therefore becomes the object of study in this work. It is proposed to evaluate the ABC in solving constrained optimization problems. The treatment to be given to violations of constraints is through penalty, which increases the objective function in the case of constraint violation. In this paper we apply an adaptive penalty method, which does not depend on user defined parameters. This approach makes the algorithm robust and more competitive.

It is proposed to evaluate the algorithm through its implementation in a set of problems of Mechanical Engineering, widely treated in the literature and present a methodology for comparison with other results in the literature.

Tuesday, July 22, 2014 - 11:00am-11:30am, 22G1
Constrained Optimization Framework for 1D Seismic Wave Propagation Problems
By Anibal Sosa
Universidad Icesi

We create a unified algorithmic framework that accommodates several constrained optimization schemes, to solve a one-dimensional (1D) inverse wave propagation problem. This framework is intended to be generally applicable. We consider the inverse problem with a PDE-constrained optimization formulation, where we invert for the material properties throughout the domain, i.e. the local wave speed. We introduce inequality constraints over the inversion parameter and treat them in turn with a logarithmic barrier, primal-dual interior-point, and primal-dual active set methods. We facilitate the implementation of these methods through a unified affine invariant approach, proposing a novel line search step computation, and ultimately identifying robust schemes that incorporate inequality constraints for solving the inverse problem. For each method, we conduct numerical experiments for synthetic example problems, where the velocity models are derived from seismic measurements, and report the behavior and performance of each method.

Tuesday, July 22, 2014 - 11:30am-12:00pm, 21G1
Formal Second-Order Accuracy Conservative Finite Difference Method for the Heat Equation
By Jhonnathan Arteaga Arispe
Universidad Simón Bolívar

In the past, a New Conservative Method for Unsteady Heat Equation have been derived by the same authors of this work. Numerical advantages and a convergence analysis was shown in a previous article, but a formal proof of the second order accuracy was not included. This work presents an elegant proof of this last issue and numerical tests which illustrate the theoretical result.

Tuesday, July 22, 2014 - 11:30am-12:00pm, 22G1
Adjoint Method for a Tumor Invasion PDE-Constrained Optimization Problem in 2D Using Adaptive Finite Element Method
By Cristina Turner
Universidad Nacional Córdoba

In this paper we present a method for estimating unknown parameter that appear in a two dimensional non-linear reaction-diffusion model of cancer invasion. This model considers that tumor-induced alteration of micro-environmental pH provides a mechanism for cancer invasion. A coupled system reaction-diffusion describing this model is given by three partial

differential equations for the 2D non-dimensional spatial distribution and temporal evolution of the density of normal tissue, the neoplastic tissue growth and the excess concentration of H^+ ions. Each of the model parameters has a corresponding biological interpretation, for instance, the growth rate of neoplastic tissue, the diffusion coefficient, the reabsorption rate and the destructive influence of H^+ ions in the healthy tissue.

After solving the direct problem, we propose a model for the estimation of parameters by fitting the numerical solution with real data, obtained via *in vitro* experiments and fluorescence ratio imaging microscopy. We define an appropriate functional to compare both the real data and the numerical solution using the adjoint method for the minimization of this functional.

We apply a splitting strategy joint with Adaptive Finite Element Method (AFEM) to solve the direct problem and the adjoint problem. The minimization problem (the inverse problem) is solved by using a trust-region-reflective method including the computation of the derivative of the functional.

Tuesday, July 22, 2014 - 3:00pm-3:30pm, 21G1

Elliptic Equations with High-Contrast Coefficients and Applications

By Leonardo Andrés Poveda Cuevas

Universidad Nacional de Colombia

In this work we show some results on the approximation of solutions of elliptic equations with high-contrast coefficients. In particular, we consider elliptic problems for which we detail the derivation of asymptotic expansions for the solutions in terms of the high-contrast value in the coefficients. We consider the case of two dimensional polygonal domains with several inclusions. We review some numerical examples and make some interesting observations.

Tuesday, July 22, 2014 - 3:00pm-3:30pm, 22G1

Second- and Fourth-Order Mimetic Discretization of 2-D Elliptic Problems on Equidistributed Grids

By Jaime Blanco

Universidad Central de Venezuela

The discretization of a continuous differential model using mimetic finite difference (MFD) presents the simple formulation and same computational efficiency as typically offered by traditional FD. However, MFD satisfy fundamental properties of vector and tensor calculus including a discrete analog of the divergence theorem, and then it follows that conservative and symmetry properties fulfilled by continuous solutions are preserved in numerical results. In this work, we apply second- and fourth-order MFD to solve elliptic problems on 2-D

rectangular meshes with adaptive variable spacing. Automatic grid adaptation allows an equidistribution of numerical errors on mimetic approximations of the solution gradient over the whole problem domain. On tests that exhibit extreme boundary layers, non-uniform MDF yield highly accurate results and show the expected convergence given by the nominal discretization. Using linear interpolation of mimetic gradient components, we also apply these MDF to full-tensor diffusion problems and observe a minor degradation of convergence rates only in the case of fourth-order discretization.

Tuesday, July 22, 2014 - 3:30pm-4:00pm, 23G1

High-Order In-Plane Rupture Simulations on Fully Staggered Grids

By Adelis Nieves

Universidad Central de Venezuela

In this work, we present a numerical method for rupture simulation on a viscoelastic medium using high order mimetic finite differences on a rectangular Fully Staggered Grid (FSG). This grid allows the representation of a geological fault by a set of compound nodes that place all stress and displacement components including split values of those discontinuous field values across this interface (under rupture propagation). A first version of this method offers consistently fourth-order accuracy for spatial discretization of the fault-viscoelastic model on the whole domain. The second approach increases the accuracy of numerical differentiation up to eight order on off-fault gridlines. We use these numerical schemes for modeling mode II ruptures on planar faults where frictional resistance is slip dependent. A preliminary convergence and dispersion analysis using as reference finite difference solutions on highly refined grids, proves the suitability of FSG for rupture dynamic simulations.

Tuesday, July 22, 2014 - 3:30pm-4:00pm, 22G1

Approach for Generating Energy Indicators in Coal Mixtures Gasification for the Analysis of the Synthesis Gas Composition

By Marlon Bastidas Barranco

Universidad de la Guajira, Colombia

An important aspect in the combustion of coal for purposes of generating clean power is to achieve that this solid fuel is gasified and hereby to capture the residues across different mechanisms and to use the gas of synthesis in the energy production. Gasification has been widely studied, but the amorphous characteristics of solid fuels causes the gasification reactions not to obey a defined order. However, it has been made possible to follow the kinetics of these reactions and orient products of synthesized gas, according to needs. In this regard, for purposes of power generation, the hydrogen production at high rates is a problem of stability of the synthesis of gas combustion. Therefore, their generation in the gasification

should be controlled by the generation of methane and carbon monoxide. The objective of this work is to provide guidance with a theoretical tool to establish the optimal mix of solid fuels in relation to the gasifying agents in order to produce a synthesized gas with appropriate levels of hydrogen. For this purpose, genetic algorithms are used solve the resulting multiobjective optimization nonlinear problem with multiple variables.

The variables that control the generation of products of synthesized gas correspond to the amount of steam and oxygen /air relative to fuel flow fed to the gasification reactor. The results show that there may be many possibilities for feeding the gasifier, but there are defined relationships that can control, with some limitations, the hydrogen production in convenient relationships with carbon monoxide.

In the third run of the multiobjective algorithm, we obtained the least amount of ash and a very high share of coal in the mix of Cesar.

Wednesday, July 23, 2014 - 9:30am-10:00am, 23G1
Analysis of Non Newtonian Blood Flow in Remodeling Radio- Cephalic Fistulas Used in Hemodialysis Process
By Janaína de Andrade Silva
Federal University of Juiz de Fora

Chronic renal failure is a disease that occurs in partial loss of kidney function, slowly progressive and irreversible. As the leading alternative treatment for this deficiency we use the blood filtering process called hemodialysis . This is a process which consists in filtering blood and removing impurities from this liquid, similar to the process executed by the kidney. The blood is first transported through a venous inlet, which is connected to an artificial artery or fistula, shortly after the blood passes through the dialysis process being filtered.

This process is extremely stressful in many cases for the patient, because there is a constant loss of venous inputs (fistulas) susceptible to this process, due to the irregularity of the tension that occurs in the blood vessel wall, developing diseases such as intimal hyperplasia. The problem related to fistula are caused by friction generated by the shear force of blood on the walls of the veins. Intimal hyperplasia is a process in which cells proliferate in the vessel inner wall in response to injury. This can reduce the useful area of the structure, hampering the passage of the blood, which can develop stenoses.

Within this context we aim to create a computational model that is able to demonstrate blood flow in fistulas, offering different angles of junctions between veins and arteries in lateral-terminals fistulas, in order to analyze the importance of remodeling of arteriovenous fistulas in the appearance of stenoses provided by intimal hyperplasia.

For this model we used near dimensions of reality, and developed and simulated with Open Foam CFD software. The governing Navier-Stokes equations were discretized with the Finite Volume Method on unstructured grids. The blood flow was considered as a Non Newtonian fluid using Carreau fluid. Two angles for arteriovenous junctions of 30 and 45 degrees were proposed . As preliminary results we observe that the main area of structure formation generated by hyperplasia are near the junction area of the graft, and the main cause of failure is in the maturation of vascular grafts for hemodialysis.

Wednesday, July 23, 2014 - 10:30am-11:00am, 21G1
An Upwind Finite Volume Method for the Convection Diffusion Equation on Non-orthogonal Quadrilateral Meshes
By Giselle Sosa
Universidad Simon Bolivar, Venezuela

The numerical reservoir simulation is an indispensable tool and widely accepted in the oil industry, because by mathematical and numerical models can simulate the flow of fluids in the reservoir, thus allowing design efficient exploitation strategies.

Traditionally, the finite difference method has been applied to solve numerically the partial differential equations governing fluid flow in porous media both for its easy implementation as computational efficiency of execution.

However, this method is in general only applied on rectangular meshes discretizing the reservoir, which do not honor its complex internal structures (preferential flow channels, faults, areas of high permeability contrast, changes in sediment type, etc.). That is why the mesh generation honoring these structures is the initial step for the simulation.

In a series of previous works, a generator of non-rectangular grids, and formed only by quadrilaterals honoring the internal structures of a reservoir and given by a set of polygonal lines was developed. This generator is based on the resolution of a system of elliptic partial differential equations using finite differences, and then the resolution of a nonlinear system of large dimension using Spectral Projected Gradient techniques type. Taking these meshes as the discretization of the reservoir, the aim of this work is to solve the two-dimensional convection diffusion equation in both steady state and transient state, taking into account different physical configurations of the porous medium. To take advantage of the good representation of the domain through these meshes, the finite volumes method was used, which is conservative and facilitates the treatment of the boundary conditions. In this method the convection diffusion equation is integrated on each quadrilateral (control volume) of the mesh, thus obtaining the integral form of the equation. The velocity value in the face of each quadrilateral is determined according to the direction of the flow (upwind scheme type).

After approximating the integrals involved and taking into account the boundary conditions, a discrete equation in each control volume showed up. Finally, a large dimension sparse linear system is obtained, generally not symmetric and ill-conditioned, which can be solved by iterative methods such as GMRES with incomplete LU preconditioning.

The boundary conditions considered are Dirichlet and Neumann type, and for both stationary and transient states. For the latter, it progresses in time, from the solution obtained in the steady state, using an implicit scheme.

Different scenarios were considered varying boundary conditions, source term, and diffusion constant fluid velocity, both in stationary and transient regime. The fluid velocity is considered moderate (low Peclet number) in all the studied configurations. The results are consistent with the physical interpretation of each configuration.

Wednesday, July 23, 2014 - 10:30am-11:00am, 23G1
Evaluation of a Heart Model Based on Cellular Automata and Mass-Spring Systems
By Ricardo Silva Campos
Universidade Federal de Juiz e Fora, Brasil

The mechanical behavior of the heart is triggered by the propagation of an electrical wave, called action potential. Many diseases have multiple effects on both electrical and mechanical cardiac physiology. To support a better understanding of the multi-scale and multi-physics processes involved in physiological and pathological cardiac conditions, a lot of research is being conducted in the development of computational tools to simulate the electro-mechanical behavior of the heart. In this work we propose a new electro-mechanical model. We have used cellular automata to simulate the action potential propagation and the force that contracts the heart. To model the mechanical tissue behavior we have used a mass-spring system. These methods were adopted since they are faster than the traditionally and commonly used models based on differential equations (DEs). In order to assess the simulation results of our model, we perform a verification with another synthetic well known model based on DEs. Preliminary results suggest that our new model was able to qualitatively reproduce the results obtained by the DEs based model with much less computational effort.

Wednesday, July 23, 2014 - 11:00am-11:30am, 21G1
Time-Splitting Scheme for Nonhydrostatic Atmospheric Model
By Andrei Bourchtein
Pelotas State University, Brazil

Complete three-dimensional models of the atmosphere have solutions of different space and time scales. The fastest atmospheric waves are the acoustic ones, which do not contain

any significant part of the atmospheric energy. The slower gravity waves are more energy valuable, while slow advective processes and Rossby waves carry the main part of the atmospheric energy. In this study, a time-splitting semi-implicit scheme is proposed for the nonhydrostatic atmospheric model, which approximates implicitly the fast acoustic and gravity waves, while slow processes are treated explicitly. Such time approximation requires solution of three-dimensional elliptic equations at each time step. Efficient elliptic solver is based on decoupling in the vertical direction and splitting in the horizontal directions. Stability analysis of the scheme shows that the time step is restricted only by the maximum velocity of advection. The performed numerical experiments show computational efficiency of the designed scheme and accuracy of the predicted atmospheric fields.

Wednesday, July 23, 2014 - 11:00am-11:30am, 23G1
Simulation of Coronary Perfusion in the Myocardium Using a Darcy Model for Fluid in Porous Medium
By João Rafael Alves
Federal University of Juiz de Fora

This paper presents the development of a computational-mathematical model to characterize the spatio-temporal dynamics of blood perfusion in cardiac myocardium. More specifically, we are interested in reproducing images obtained by magnetic resonance imaging (MRI) with contrast images, which are widely used in medical practice for the assessment of blood perfusion in the heart. The application of contrast enable the detection of lesions, ischemic regions, fibrosis or tumors through the noninvasive MRI. In our modelling, we treat the myocardial tissue of the heart as a porous medium, i.e., a solid region with empty spaces. To this end, we made a model based on differential equations in a two-dimensional domain and using the Darcy Law, which correlates tissue permeability, pressure difference and the blood flow in the heart. The mathematical model was solved by a decoupling of operators. The resolution of the first stage provides the spatial distribution of pressure and velocity throughout the domain. Knowing the velocity field, then it is used in the second stage, based on the solution of an advection-diffusion equation where the variable (temporal and spatial) is the contrast. For the discretization of the equations, the Finite Volume Method was used. Different tests were made ranging the cardiac fiber directions (anisotropy) and also the location and size of ischemic region in a two-dimensional model of cardiac tissue. In a future work we intend to validate the models by comparison between the simulations and medical images obtained by MRI.

Wednesday, July 23, 2014 - 11:30am-12:00pm, 21G1

Modeling Three-Dimensional Winds in Ensenada, Baja California Region

By Carlos Torres

Mexico National Oceanographic Data Center & Institute for Oceanological Research/UABC

This study presents numerical simulations of observed flows impinging upon topography representative of the Ensenada region. We conducted a series of numerical experiments using the General Curvilinear Atmospheric Model (Torres et al. 2014). Simulations with 100m horizontal grid resolution were performed for most persistent winds. We evaluated the model using measured data, and the simulated wind fields were used to compute the wind stress and other variables of interest.

Wednesday, July 23, 2014 - 11:30am-12:00pm, 23G1

Computational Modeling of Immune Response to Infection by Yellow Fever Virus

By Carla Rezende Barbosa Bonin

Federal University of Juiz de Fora

Yellow fever (YF) is an infectious disease caused by a type of virus called flavivirus. The disease is transmitted when a mosquito bites an infected person or other primate and then bites a healthy person who is not immune. In the world, 44 countries are endemics, mainly in Africa and South America, and the World Health Organization (WHO) estimates 200,000 cases of YF per year, causing 30,000 deaths [1]. There is no specific treatment for YF, the treatment is based on supportive clinical management to ease the symptoms. The best way to prevent YF is the vaccination.

Currently available YF vaccines are based on attenuated live virus of the 17D lineage. At the moment, a booster dose of YF vaccine should be administered each 10 years but, according to WHO, a single dose of YF vaccine is sufficient to confer sustained life-long protective immunity against YF disease [1]. Although there are no prospective clinical studies on the durability of efficacy of the YF vaccine in humans, distinct studies have shown that there is evidence to support the recommendation of the WHO [2, 3, 4, 5].

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o better understand the behavior of the disease and the vaccine it is necessary to understand the behavior of the immune system. To this end, this work presents a mathematical model of the immune response to an infection caused by the YF virus. To the best of our knowledge this is the first mathematical model of the effects of the YF in the immune system. This model was based on a previous work [6], which reproduces the effects of influenza A virus infection. The original model was modified with the rearrangement of some populations and modification of some equations and parameters so that it could reproduce,

for example, the behavior of the YF virus in the organism from infection until the removal of it by the immune system cells. The model takes into account both the innate and the adaptive immune system cells and molecules, such as dendritic cells, T cells, and B cells and antibodies. This model will allow us, in future works, to reproduce the effects of the vaccine in the body, allowing us to verify, for example, if a booster dose of YF vaccine is really necessary every 10 years.

Wednesday, July 23, 2014 - 2:00pm-2:30pm, 21G1

Hiperbolicity and Implementation of the WENO Spectral Method with Adaptive Multi-Resolution for the Lighthill-Whitham-Richards Traffic Model

By Edwin Alberto Bolaño Benítez

Universidad del Norte, Colombia

In this paper we describe in detail the implementation of a spectral or characteristic-based fifth order WENO (Weighted Essentially Non-Oscillatory) scheme along with an adaptive multiresolution technique for computing efficiently the numerical solution of a multi-class traffic flow model described mathematically by a nonlinear system of conservation laws. R. Bürger, A. Kozakevicius considered the same problem but in a component-wise manner. Later, R. Donat, P. Mulet included spectral information but using the AMR (Adaptive Mesh Refinement) technique instead of multiresolution based schemes.

Wednesday, July 23, 2014 - 2:00pm-2:30pm, 23G1

Simulations of the Anisotropic Electrical Activity of the Heart Using the Lattice Boltzmann Method

By Joventino Oliveira Campos

Federal University of Juiz de Fora

Computational modeling has been used for understanding complex phenomena in various areas of science recently. In particular, mathematical models of the electrical activity of the heart has received great attention from the scientific and medical community. These models allow a better understanding of complex biophysical phenomena, the development of new techniques for therapy and also serve as a platform for drug tests.

The cardiac electrophysiology may be simulated by solving a partial differential equation coupled to a system of ordinary differential equations describing the electrical behavior of the cell membrane. The numerical methods most commonly used to solve these problems are the finite element method (FEM) and finite volume method (FVM). A recent alternative is the Lattice Boltzmann Method (LBM), which has been successfully used for simulation of complex problems in fluid dynamics.

This work presents the lattice Boltzmann method for computational simulations of the cardiac electrical activity using Monodomain and Bidomain models. Instead of using the traditional collision operator BGK from LBM, a model with multiple relaxation parameters known as MRT, was applied in order to consider the anisotropy of the cardiac tissue. The proposed model is evaluated using a benchmark problem and also under irregular and complex 3D domains. Due to the inherent high level of parallelism present in the LBM, results from the use of GPUs for the acceleration of the computational simulation will be presented.

Wednesday, July 23, 2014 - 2:30pm-3:00pm, 21G1

Comparative Evaluation of Three Tsunami Models: Goto-Ogawa, GEOCLAW and Delft3D for the 1867 Virgin Islands Scenario and its Effect on the Western Venezuelan Coast

By Manuel Valera Arriojas

FUNVISIS, Venezuelan Foundation for Seismological Research

Tsunami numerical simulation has become a powerful tool for decision making in an event of a Tsunamigenic earthquake. However, for the Caribbean there are no historical sea level records to validate those models. Therefore, model errors are currently inevitable, due to uncertainties in the initial, boundary conditions and bathymetry, as well as in the oversimplified or entirely neglected physical processes. In this sense, and for Tsunamis simulation particularly, different methods exist to solve the shallow waters equation, while each kind of solution presents numerical errors. In this work, a sensibility analysis is presented for three numerical models: Goto-Ogawa (supported by UNESCO), Delft3D and GeoClaw, using as the study case the 1867 Virgin Islands Tsunami, according to the parameters of the UNESCO exercise Caribe Wave 2011, with impact on Venezuelan coasts, specifically in the Nueva Esparta State. Synthetic water level time series from several locations around the Venezuelan eastern coast are obtained from the different models and compared with the maximum wave height reported historically for its validation. The goal of this work is not to select the best possible model, but to take advantage of the best of each one, to obtain the best estimation of maximum height and arrival times of the tsunami to Venezuelan coasts.

Wednesday, July 23, 2014 - 2:30pm-3:00pm, 23G1

On Generation of Spatial Grids for Numerical Models of Geophysical Flows

By Natalia Naoumova

Pelotas Federal University, Brazil

Generation of the computational grids is one of the important elements for definition of the features of a numerical scheme. If a high precision numerical solution is required over all the considered domain, which is the standard situation in regional atmospheric and ocean modeling, then the computational grid should be as physically uniform as it is possible in order to guarantee the highest accuracy and stability of the dynamic part and the most justified choice of the parameterization schemes for the physical part of the numerical model.

Simulation of large-scale atmospheric and ocean processes, such as weather phenomena, regional and global circulations, and climate dynamics, imply the formulation of the corresponding models in spherical geometry. The use of the natural geographical coordinates leads to generation of highly non-uniform computational grids. One of the widespread approaches to circumvent this problem is the application of conformal mappings from a sphere onto a plane. In this case, the problem of generation of computational grids with the minimum possible physical distortion can be formulated in terms of minimization of the variation of the mapping factor over a chosen domain. In this report we present the results of the generation of rectangular grids for the spherical regions of different sizes and forms and compare the obtained results for practical computational grids with theoretical evaluations.

Wednesday, July 23, 2014 - 3:00pm-3:30pm, 21G1

The Simulation of the Hydrodynamics of the Urias Estuary in Mexico

By Isabel Ramirez

Centro de Investigación Científica y de Educación Superior de Ensenada

Estero Urias is a coastal lagoon, sited in the Pacific coast of Mexico (23.21° N, 106.39° W), 7 kilometers long and an L-shape. The estuary has 7 main inflows discharging in the lagoon. The bathymetry is regular in the first two kilometers, which is used as a port. This zone is 13 meters depth ending in the corner of the L shape. After this zone, the bathymetry becomes irregular with a main channel and shallow areas of 2 meters depth. Sea level and meteorological data were used to force a three-dimensional hydrodynamic model with good results. The results are validated with currents and temperature data at the entrance of the estuary showing a correlation of 0.75. Additionally the model results give information of the circulation of the estuary waters on places difficult to measure.

Wednesday, July 23, 2014 - 3:00pm-3:30pm, 23G1

Model of the Population Dynamics of Lutzomyia Longiflocosa, Vector of Cutaneous Leishmaniasis in Colombia

By Gelys Mestre

Universidad de La Salle, Colombia

Leishmaniasis is a disease of great public health importance in Colombia. However, knowledge of insect vectors is very limited. *Lutzomyia longiflocosa* is the vector involved in the major epidemics recorded in recent years in the country. Key factors for prevention and vector control, as abiotic and biotic determinants of the vector abundance, are poorly understood. Knowledge of the above determinants together with the generation of a population dynamics model for *L. longiflocosa* could improve the understanding of the biology and ecology of this sandfly species. The model could contribute to the development of prevention and control programs. Particularly, the model could be used to predict the times of high risk of transmission for cutaneous leishmaniasis and to simulate the effect of control measures prior to their implementation.

The association between climatic factors (rainfall and temperature) and the abundance of adult *L. longiflocosa* in the sub-Andean region of Huila is tested using generalized linear models. Based on the identified factors, its parameters, plus the available bibliographic information on the life cycle of *L. longiflocosa*, a deterministic population dynamics model has been generated.

Rainfall was identified as one of the climatic determinants of the abundance of *L. longiflocosa*. The time lags of this variable, associated with the high abundance peaks of this sandfly, was identified. The population dynamics model was consistent with the observed density of *L. longiflocosa* recorded in a previous work within the study area.

The developed mathematical model provides a starting point for understanding the population dynamics of *L. longiflocosa* that can be incorporated as a tool in the control of leishmaniasis.

Wednesday, July 23, 2014 - 3:30pm-4:00pm, 21G1

A FEM-Based Study on the Influence of Skewness and Kurtosis Surface Texture Parameters in Human Dental Occlusal Contact

By Evelyn Aparecida de Oliveira

Federal University of Juiz de Fora

Wear of human teeth is an irreversible condition that occurs with different severity and may lead to loss of integrity and functionality. As dental wear is a contact problem, it is important to investigate the surface quality using quantitative methods. Despite the variety of available tests for measuring surface

changes, two statistical variables are the most commonly reported in experimental studies: roughness average and root mean squares (RMS) deviation. Nonetheless, profilometry allows to estimate other statistical parameters of a surface: skewness, the measure of the asymmetry of surface deviations considering a mean plane; and kurtosis, the measure of the peakedness, or sharpness, of the height distribution topography. The approach used to simulate the contact between rough surfaces, given the probability density functions, consists in discretizing them into several intervals, so that each one represent a main asperity. The deformations of the main asperities are analyzed and using homogenization techniques it is possible to establish the relationship among the responses that have occurred in micro-scale and the predicted responses in macro-scale. In this work we created parameterized scripts in Python language for the Abaqus CAE software in order to analyze the influence of skewness and kurtosis on numerical results for contact of human dental surfaces. We performed four sets of experiments: varying mean roughness, mean peaks curvature, skewness and kurtosis of asperities distribution. The graphical user interface of ABAQUS/CAE module was used to create a model example of contact between an asperity and a rigid plane, and the commands were issued internally by ABAQUS/CAE after each operation and recorded in a script type file in a object-oriented programming language called Python. This file was accessed and parameterized according to the variables of the problem, mainly to include a loop to repeat the modeling tasks and access to the data output for each main asperity considered. A function to assist in the automated generation of geometry based on the texture parameters was defined, which calculates a list of the coordinates of a number of points located on the asperity slope. The script contains all native commands of Abaqus/CAE module, but parameterized. The contact forces and areas for each increment were accessed from the database output and written in the form of a report. After recording all reports, a routine, also in Python, was responsible for reading them successively, calculating the expected total values for the interface, taking into account the contribution of each main asperity. Using the library matplotlib, the final curves were plotted. The goals were to verify whether a combination of skewness and kurtosis parameters help us to explain clinically studied cases of dental wear.

Wednesday, July 23, 2014 - 3:30pm-4:00pm, 23G1

Reverse Engineering of 3D Point Clouds by Means of Curved Triangular Patches

By Gudrun Albrecht

Université de Valenciennes

Problems of “Reverse Engineering” type are recurrent in Computer Aided Design (CAD) and in computer graphics, in general. They consist in the reconstruction of objects from point clouds. In computer graphics, for visualization purposes, for example, the existing solutions consist in triangulating the

point data and then fitting them with planar triangles. The object is thus approximated by a piecewise linear surface, which is only C0 continuous. In order to obtain a smooth aspect a huge amount of triangles is necessary. Triangular meshes are widely used because they are sufficiently general to represent surfaces of arbitrary genus.

This talk deals with scattered data interpolation methods by means of polynomial and rational parametric surfaces in Bezier form of the lowest possible degree. Two different approaches are dealt with:

- on the one hand we present a new G1 rational blend interpolatory scheme, i.e., a method that uses rational blends to construct the surface avoiding the so-called vertex consistency problem (authors: G. Albrecht, F. Calio, E. Miglio);
- on the other hand we focus on a geometric construction of single rational parametric triangular quadratic patches which lie on quadrics. The resulting quadric design element offers three free shape parameters and is useful for reverse engineering applications dealing with objects from mechanical engineering and architecture that contain a large amount of “quadric” shapes (authors: G. Albrecht, M. Paluszny, M. Lentini, S. Posada).

Wednesday, July 23, 2014 - 4:30pm-5:00pm, 21G1
A Singular Value Decomposition-Based Method to Parameterize Three-Dimensional Models Used to Estimate Cardiac Ejection Fraction by Electrical Impedance Tomography

By Marcos Henrique Fonseca Ribeiro
Federal University of Juiz de Fora, Brazil

Cardiac Ejection Fraction (EF) is an important parameter to analyze heart efficiency as a pump and it is clinically correlated to the functional status of such organ. Among the diverse techniques that can be used to determine or estimate EF is Electrical Impedance Tomography (EIT), which presents advantages over the alternatives, mainly because of its low operational costs, high portability and the fact that it can be used to frequently monitor this clinical important parameter. The goal of EIT is to reconstruct conductivity distribution images of the interior of a conductor domain. This can be accomplished by applying electric currents on the boundary of the domain and measuring the electrical potentials obtained also on the boundary of the body. Such problem can be mathematically classified as a non-linear inverse problem, and it can be addressed as an optimization or a classification/regression problem. An important issue of this problem is the representation of the geometric features of the models that represent each one of the regions of interest in our study, because this has a high influence on the computational costs of the techniques used to solve the inverse problem. In this work, we propose an approach that deals with three-dimensional models for the regions of interest,

obtained by semi-automatic segmentation performed over Magnetic Resonance images. The resulting geometry of the models are represented by polygonal meshes that are compacted into a parameterized representation. The parametrization proposed is based on a Principal Components Analysis (PCA) performed using a Singular Value Decomposition (SVD) over matrices composed by geometrical and/or both geometrical and electrical data of various different stages of the heart obtained by previous simulations. The parameterization of the geometries aims at the decrease of the overall computational cost of the inverse problem technique by reducing the number of optimization variables, since the local searches performed by the optimization technique are based on the continuous distortion of the meshes for the heart ventricles. Therefore, to decrease the number of optimization variables (geometric parameters), it is an important aspect for the study of the EIT problem applied to the determination of Cardiac Ejection Fraction. We present two similar, but different approaches for the parameterization and both are tested using a hybrid heuristic to solve the mentioned inverse problem. Our heuristic uses the solution of the direct problem associated to EIT, by means of the Boundary Elements Method (BEM), and Support Vector Machines for Regression (SVR), to estimate initial guesses for the technique, and then uses the metaheuristic called Iterated Local Search (ILS), to manage multiple Levenberg-Marquardt Method (LMM) executions, which work as local searches inside the proposed schema. The results presented for experiments performed on synthetically generated data for electric potentials are discussed, together with some directions for future studies and for the sophistication of the model, as well as other important aspects of the addressed problem.

Wednesday, July 23, 2014 - 4:30pm-5:00pm, 23G1
Three Dimensional Mimetic Operators on Non Uniform Rectangular Grids
By Jaime Blanco
Universidad Central de Venezuela

In this work, we generalize the Castillo-Grone mimetic gradient and divergence finite difference operators to three dimensions, which combined to a boundary flux operator satisfy an extended Green's theorem in the discrete sense. Consistency of the resulting discrete Laplacian is formally proven in the context of general Robin's boundary conditions. We also study the numerical convergence of second- and fourth-order mimetic discretizations of oil reservoir simulation problems. Strong singularities on the source injection terms require adaptive grid spacing to efficiently resolve high solution gradients. Thus, we adapt these operators to 3-D rectangular grids with variable spacing to automatically equidistribute numerical errors on the gradient approximation along the whole domain.

Wednesday, July 23, 2014 - 5:00pm-5:30pm, 21G1
Analysis of a Family of Linear Degenerate Parabolic Mixed Equations
By Ramiro Acevedo
Universidad del Cauca, Colombia

The aim of this talk is to show an abstract framework to analyze a family of linear degenerate parabolic mixed equations. We combine the theory for the degenerate parabolic equations with the classical Babuska-Brezzi theory to deduce necessary and sufficient conditions to prove the well-posedness of the problem. Finally, we show two recent mixed finite element formulations which arise from electromagnetic applications and deduce their well-posedness by using the developed abstract theory.

Wednesday, July 23, 2014 - 5:00pm-5:30pm, 23G1
Advances in Multiple Burst-Correcting Codes
By Ana Lucila Sandoval Orozco
Universidad Complutense de Madrid, Spain

In many communication channels, noise disturbances tend to occur in the form of bursts. Channels modeled by Gilbert [1] and Elliot [2] fall into this category. Under these circumstances it is not efficient to use random-error-correcting codes. Codes capable of correcting multiple burst are efficient tools of error control for such channels. Some new bounds are presented for multiple burst-correcting codes that extend the previously known bounds, such as the Reiger [3] and the Gallager [4] bounds. It is shown that both the new bounds coincide for block codes. For some values, the new bounds improve the extended volume bound.

Wednesday, July 23, 2014 - 5:30pm-6:00pm, 21G1
An Adaptive Uzawa Method for the Steady Stokes Equation
By Catalina Maria Rua Alvarez
Universidad de Nariño

The present work is motivated by the study of incompressible flows at low Reynolds numbers. In the limit, as the Reynolds number approaches to zero, the dynamics of the system is modeled by the steady Stokes equations. An adaptive version of Uzawa Method is proposed to solve those equations with Dirichlet boundary conditions on locally refined grids.

Adaptive mesh refinements increase locally the resolution of the method to improve accuracy at low computational cost. A finite difference approach is used for the discretization of the fluid velocity in a staggered fashion and Uzawa Method is employed to handle the pressure-velocity coupling in primitive variables. To solve the resulting set of algebraic equations, the matrix representing the discretization on the adaptive grid is built and the related linear system solved by PETSc (Portable, Extensible

Toolkit for Scientific Computation) library. Several methods are tested for their performance, including the biconjugate gradient and GMRES methods, with suitable preconditioners. The parallel capabilities are investigated.

Wednesday, July 23, 2014 - 5:30pm-6:00pm, 23G1
An Efficient Algorithm for Searching Optimal Multiple Burst-Correcting Codes
By Ana Lucila Sandoval Orozco
Universidad Complutense de Madrid, Spain

In many communication channels, noise disturbances tend to occur in the form of bursts. Channels modeled by Gilbert [1] and Elliot [2] fall into this category. Under these circumstances it is not efficient to use random-error-correcting codes. Codes capable of correcting multiple burst are efficient tools of error control for such channels. An efficient algorithm searching for the best (shortened) cyclic multiple burst-correcting codes is presented. The algorithm is based on Gray codes and extends a previous one [3] [4] for searching one-burst correcting codes. The efficiency of the algorithm stems from the fact that no repeated syndromes are computed.

Thursday, July 24, 2014 - 9:30am-10:00am, 21G1
Mimetic and Standard Finite Difference Approaches to Modeling the Diffusion of Calcium Within a Single Sarcomere of an Adult Cardiomyocyte
By Rosa Lemus
San Diego State University

How does free calcium ion flow occur through the sarcomere (the repeating contractile unit of myofibrils within the cardiocyte) in triggering contraction? We wanted to visualize this process in an animation to best appreciate the pattern of calcium flow within a muscle cell using mimetic methods to calculate the concentration of calcium. We focused on the role calcium ions play during the excitation-contraction coupling process, including on the expression of genes that serve in calcium transport across cell membranes (outer membrane and the SR). We created a mathematical model to demonstrate the calcium turnover, and the dependence upon factors like abundance and transport rates of RyR2, SERCA2 and NCX channels.

The model will be solved using mimetic finite difference (MFD) methods and standard finite difference (SFD) methods with MATLAB implementations for visualization. Assuming radial symmetry in a cylindrical sarcomere, a 2D grid model accounts for calcium exchanges within the myofilament system, between the SR's terminal and longitudinal cisternae, and within the cytosol. A 2D sarcomere was divided into computational cells. The rate of Ca^{2+} release from the terminal cisternae (TC) region was assumed to be proportional to the product of the number of

open Ca^{2+} release channels and the difference of $[\text{Ca}^{2+}]$ between the TC and a cell facing the TC. Ca^{2+} moves from element to element by simple diffusion and is taken up by the longitudinal SR via the SERCA2 pump. Ca^{2+} influx responsible for triggering the TC Ca^{2+} release is introduced to elements at the level of the Z-line. Calcium buffering is considered for a more realistic model. We take into account calcium binding to troponin C (TnC) found on the thin myofilaments and calmodulin (CaM) found ubiquitously in the cytosol.

An animated visualization of the fluxes will use pseudocolor to represent the calcium concentration changes vs. time in the sarcomere during a single twitch. We anticipate that increases in SERCA2 channel density cause a faster relaxation rate of the Ca^{2+} transient. Changes in number of RyR2 and NCX channels should alter Ca^{2+} transient amplitudes and kinetics in a manner predicted by our laboratory's gene silencing experiments.

The schemes for the MFD and SFD methods will be second order accurate. For preserving second order accuracy about the boundaries of our computational domain, the SFD method uses ghost values for the approximations. The MFD method does not use ghost values or extrapolation, but instead computes the values at the boundaries and would provide a closer approximation of the physical values about the boundaries. The two methods are used for comparison purposes.

Future work of a finished simulation may examine other features relating to calcium fluxes such as a more detailed description of the Ca^{2+} -induced Ca^{2+} release mechanism. The model may be extended to represent a whole adult cardiomyocyte and account for other sites of calcium buffering. Higher order accuracy may also be implemented by the use of more points per approximation for both methods.

Thursday, July 24, 2014 - 10:30am-11:00am, 22G1
Variational Methods for Meshless Approximation of Surfaces: Comparing the FEM
By Alberto Hananel Baigorria
Universidad de Granada/Universidad Católica Santo Toribio de Mogrovejo

In Earth science, especially Geology and other Sciences and Technologies, the reconstruction of surfaces from some scattered data set is a commonly encountered problem.

In this work, under a generic schema, we enrich the theory of the discrete variational spline functions by minimizing some quadratic functional in a suitable space which can be a fairness functional, the flexion energy of a thin plate or others.

It is essential to consider a finite dimension space of functions, where the minimization problem can be solved, and then the

variational problem will be formulated. The discrete finite dimension space of functions that we propose, in this case, is a parametric finite dimensional space generated by a radial function basis. Then, we describe a meshless approximation method of surfaces. The convergence of the problem is shown and finally, we analyze some particular examples in Geology, CAGD, Medicine and Dentistry making a comparison with FEM.

Thursday, July 24, 2014 - 10:30am-11:00am, 21G1
Mimetic Methods for Welding Plates Problems
By Giselle Sosa
Universidad Simon Bolivar, Venezuela

The welding plates problems in engineering introduce nonlinear boundary conditions of source type, when modeling numerically the temperature distribution in the material. The numerical methods traditionally used for solving this kind of problem (finite differences, finite elements, etc.) do not represent correctly the heat transfer in the welding zone. Therefore to efficiently solve this problem, a numerical method that simulates adequately the nonlinear boundary condition is required. One such method is the mimetic method. In this work we propose to use the 2D mimetic method to solve the welding plates problem with nonlinear boundary condition of source type.

Thursday, July 24, 2014 - 11:00am-11:30am, 22G1
A Least Squares Warping Algorithm for PP/PS Reflectors Matching in Pre-Stack Depth Migrated Images
By Miguel Dumett
San Diego State University

This paper presents a one-dimensional warping operator for matching reflectors present in PP and PS pre-stack depth migration (PSDM) images. It is one-dimensional because it deforms (stretch/compress) a PS-trace to look like the corresponding PP-trace. Reflector matching occurs via the construction of a delta depth map. The delta depth map is built after a convolution operator between PS- and PP-trace is estimated by a least squares procedure. Even though a deformation operator that matches PP and PS PSDM images should be at least two-dimensional or three-dimensional in nature, the present warping methodology behaves well when the deformation between PSDM images is small. The extension to two- and three-dimensions is not only straightforward but also their parallelization is simple. Since matching reflector locations does not require all-frequency content of the PSDM images, in the two- and three-dimensional cases, low-frequency versions of them might be matched instead, avoiding the need of parallelization. The warping algorithm assumes that the PSDM images illuminate the same geological events. Preliminary results with synthetic data are shown. This is a work in progress.

Thursday, July 24, 2014 - 11:00am-11:30am, 21G1

A Parallel 3D Numerical Simulation of Hyperthermia Cancer Treatment Considering a Nonlinear Bioheat Transfer Model

By Ruy Freitas Reis

Universidade Federal de Juiz de Fora

The hyperthermia technique has been widely used in cancer treatment to destroy tumors. Hyperthermia consists of applying heat at a specific area, like a tumor, to destroy cells by necrosis. Techniques based upon magnetic nanoparticles to generate heat while a magnetic field is applied have been shown to be quite effective. In this presentation, a 3D numerical nonlinear bioheat transfer model considering skin, fat and muscle tissue layers in addition to the tumor is used. The problem is modeled by the well-known Pennes' equation and a temperature-dependent blood perfusion is adopted to yield more accurate results for the hyperthermia process. The FDM in a heterogeneous medium is employed and the resulting system of nonlinear equations in the time domain is solved by a predictor-multicorrector algorithm. Since the three-dimensional model requires a large amount of computational time, this work also presents an initial attempt of parallelization using a compute unified device architecture (CUDA) in order to improve the computational performance.

Thursday, July 24, 2014 - 11:30am-12:00pm, 22G1

Compact Finite Difference Modeling of 2-D Acoustic Wave Propagation

By Luis Cordova

Universidad de Oriente, Venezuela

In this work, we implement and compare two compact finite difference (CFD) methods to solve the velocity-pressure system associated to acoustic motion on a rectangular medium. In the first method, spatial discretization proceeds on a nodal grid and leads to an implicit FD formulation to update the acoustic pressure on the whole domain. We use the alternating direction implicit (ADI) scheme to solve this formulation along each coordinate direction in a decoupled fashion, reducing the computational cost of this method. On the other hand, the design of the second method employs a novel set of mimetic CFD operators for explicit differentiation on staggered grids, which leads to a discrete formulation without having to solve a linear system. Time integration is performed by the traditional fourth-order Runge-Kutta scheme in both CFD methods. Comparison of these methods includes experimental convergence and CPU consumption on several numerical tests.

Thursday, July 24, 2014 - 2:00pm-2:30pm, 22G1

Numerical Analysis of the Acoustics of a Diffusion Flame

By Charles Quevedo Carpes

Universidade Federal do Pampa

The combustion is present in many kinds of industries. Among the various applications, gas turbine combustors are a common example of use of combustion in the industry. These devices work with high rates of energy conversion and it is important that the flame remains stable even in the presence of vortices. Any instability can blow out the flame, or increase much the production of nitrous oxides. Furthermore, the thermoacoustic coupling can generate oscillations in pressure, which may increase with time due to a feedback caused by the release of heat and the interaction with the walls of the combustion chamber. The pressure variations also produce vibration in the combustion chamber and these vibrations can decrease the lifetime and result in failures in such equipment. Therefore, efficient control of this process allows a cheaper and safer operation. However, combustion is a complex physical phenomenon that involves many factors that influence each other. To investigate the acoustic behavior of a flame is necessary to consider various characteristics such as type of flow (laminar or turbulent), type of flame (diffusive or pre-mixed) and fuel type. In this paper, we consider a turbulent diffusive flame of methane inside a combustion chamber. To model this problem we use the Navier-Stokes equations to describe the fields of velocity coupled with the differential equations that describe the reaction of methane combustion and with a wave equation to consider the pressure variation generated by the turbulent flow and the heat release from the chemical reaction. These equations are solved numerically using the finite difference scheme with a fourth-order approximation in space and third order in time. Large-eddy simulations (LES) of the flow are realized based on the Runge-Kutta multistage scheme for time integration. The model considers a 3D rectangular combustion chamber where the fuel is injected in the left and the products of combustion have free exit at the right side of the chamber. Three computational meshes are tested to obtain error estimates and the results are compared with experimental data showing good agreement. Considering the high costs for obtaining experimental data, the proposed model is a fast and an inexpensive alternative to analyze the behavior of confined flames and to estimate parameters of stability control, which are the principal contributions of this work.

Thursday, July 24, 2014 - 2:00pm-2:30pm, 25G1

Estimation of Error and Adaptivity in Mimetic Methods

By Giovanni Calderón
Universidad de Los Andes

In this paper a novel adaptive process to define an optimal mesh to compute the solution of problems using mimetic numerical methods is presented. The error estimate is based on the discrete version of the gradient operator. The numerical experimentation reveals the good performance of the method when applied to one-dimensional boundary value problems.

Thursday, July 24, 2014 - 2:30pm-3:00pm, 25G1

Data Assimilation for an Operational System in the Bay of San Quintin

By Mariangel Garcia
San Diego State University

Uncertainties in model parameters can be estimated through automated calibration by tuning a set of parameters that are fixed in time. Delft3D Model was implemented in the study of the hydrodynamics of San Quintin Bay; calibration and validation was successfully done on previous research. However, uncertainties that propagate through simulations of the future are mostly unknown, and was not tested in this region. Here is where Data Assimilation (DA) techniques play an important role. The mathematical methods of DA describe algorithms for combining observations of a dynamical system, a computational model that describes its evolution, and appropriate prior information. The aim of this work is to make a comparative analysis of the calibration methods vs Data Assimilation, as well as evaluating the long term predictive capability of the model by using water level, temperature and salinity measurements from different locations along the bay. On this aspect OpenDA is considered as a tool to deliver real time forecasting by introducing an Ensemble Kalman Filter algorithm. It is expected that the automatic procedure will result in an improved model forecast. Furthermore, it should provide information on the uncertainty of the results, which is important for drawing conclusions from simulations. On the other hand, a new computational challenge has to be addressed in order to reduce the cost of this implementation.

Thursday, July 24, 2014 - 3:00pm-3:30pm, 22G1

Numerical Analysis of Methane Combustion in Porous Media

By Elisângela Pinto Francisquetti
Federal University of Rio Grande do Sul

Currently, a large portion of the production of world energy still comes from the burning of conventional fuels, such as coal, oil, and natural gas, among others. Although climate change calls for drastic alternatives, probably combustion processes will continue to be the main form of energy conversion during decades. Furthermore, it is known that the porous matrix enhances heat from the post-flame to the pre-flame zone, due to the transport of energy by radiation and conduction, which are larger than that occurring in free flames. The numerical analysis of combustion in porous media has gained prominence in recent years due to the large number of applications of porous burners, since the use of porous material burners proved to be an efficient way to reduce emissions of the pollutants, such as NO_x and CO. For applications in combustion, the porous material must withstand high temperatures and, therefore, materials such as alumina, ceramic, silicon carbide and zirconia are used in these applications. However, it does not exist in the literature a standard model able to predict the flow characteristics for all situations.

In this paper, we present a model which is sufficiently complete to allow the analysis of combustion in porous media. The purpose of this paper is to validate this model for the premixed combustion of methane and air in porous media (zirconia), considering that the flow is steady, laminar, incompressible, and two-dimensional. The set of equations for this problem consists of the equations of momentum, energy of the gaseous phase, energy of the solid phase and mass fraction of each species. The chemical processes are described by a one-step reduced mechanism that is coupled with the other equations. The discretization in space is a second order finite difference scheme. An estimate of the discretization error is done to compare the efficiency of two classical integration methods: Gauss-Seidel and Runge-Kutta. Numerical tests are carried out for Reynolds numbers equal to 300, Zel'dovich equal to 10, Schmidt equal to 1, Prandtl equal to 0.7 and Damköhler equal to 200. The results compare favorably with data from the literature.

Thursday, July 24, 2014 - 3:00pm-3:30pm, 25G1

K-Exponential Statistical Manifold Modeled on Orlicz Spaces

By Héctor Román Quiceno Echavarría
Instituto Tecnológico Metropolitano

Given a probability measure μ , on the space of strictly positive densities $\mathfrak{M}_\mu$, we construct a topological manifold on which the elements are connected by k -exponential models in the form $q = e_k^{u \ominus K_{p,k}(u)} p$, where $p, q \in \mathfrak{M}_\mu$, and their local representations are elements of an Orlicz space, i.e the manifold is modeled on Orlicz spaces. Parameter

k is the G. Kaniadaki's parameter for k -deformed exponentials which is of strong importance on relativity and statistical complex models on statistical mechanics. Functional $K_{p,k}$ is the deformed counterpart of the cumulant mapping and satisfy that if $k \rightarrow 0$, we obtain the usual cumulant functional of the exponential manifold, moreover in this limit case the exponential manifold constructed by Pistone and Sempi is recovered. In the context of deformed exponentials, we prove that the function $\phi_k(\cdot) = \cosh_k(\cdot) - 1$, is a Young function and generates the Orlicz space on which the k -exponential manifold is modeled, namely $L^{\phi_k}(p \cdot \mu)$. This construction differs from the one made by Pistone on the paper *k-exponential models from the geometrical viewpoint*, since this last one is based on divergence functionals and modeled on Lebesgue spaces $L^{\frac{1}{k}}(p \cdot \mu)$. The use of k -deformed models is interesting since they generalize the exponentials models and extend them to non-additive systems.

Thursday, July 24, 2014 - 3:30pm-4:00pm, 22G1
Analysis of a Model Developed for Reactive Flow in Porous Media
By Elisângela Pinto Francisquetti
Federal University of Rio Grande do Sul

The reactive flow analysis in porous media has been gaining attention in recent years. One reason for this interest is its application in many areas, such as in geophysical problems, in heat exchangers, in natural convection flows of groundwater, in processes of chemical separation, in dispersion of chemical contaminants in the soil, among others. There is a strong need in petroleum geology of predicting the migration of hydrocarbons, a typical case of fluid flow in porous media.

Therefore, it is necessary to have a good knowledge of hydrological conditions of the present and the past, as well as to understand the physical processes that lead to the formation of oil in sedimentary layers, to ensure that the operation happen efficiently. Fluid flow in sedimentary layers induces reactions of precipitation and/or dissolution of carbonates, as there are large variations of thermodynamic properties and the effects of salinity and humidity are responsible for changes in the density of geo-fluids. Moreover, the flow of water in basins and the transport of solids in solution may also cause dissolution and/or precipitation of minerals, which directly influences the porosity and the permeability of the reservoir rocks. The reactive transport in Earth Sciences has become a highly multidisciplinary research area, including areas such as geochemistry, geology, physics, mathematics, chemistry, hydrology and engineering.

This paper develops a mathematical model for the reactive flow in porous media. The model is based on the dimensionless equations of momentum, energy equation, equations of concentrations of chemical species and the equation for the pressure. First, the analysis of the existence of the solution to the set of equations based on Faedo-Galerkin method is developed. After that, the set of equations is discretized by the finite difference method. The system is integrated in time by the Runge- Kutta simplified multi-stage scheme. We analyze

the discretization error due to the computational mesh through Richardson extrapolation. The tests are performed considering the reactions of dissolution and/or precipitation for the mineral calcite. The results compare favorably with data found in the literature, so that this work provides a significant contribution to a better understanding of the reactive flow in porous media.

Thursday, July 24, 2014 - 3:30pm-4:00pm, 25G1
Using Weak Forms to Derive Asymptotic Expansions of Elliptic Equations with High-Contrast Coefficients
By Sebastian Huepo Beltran
Universidad Nacional de Colombia

We consider the stationary heat equation in a high-contrast binary composite material. We are interested in the effect on the solution due to the different properties of the material. For this aim we study asymptotic expansions of the solution in terms of the ratio of the heat conductivity of different materials. We present in a detailed manner the deduction of asymptotic expansions for one dimensional elliptic equation modeling stationary heat diffusion on high-contrast composite materials. In particular we present a detailed example of an expansion and some related ideas.

Thursday, July 24, 2014 - 4:30pm-5:00pm, 22G1
Temperature and Water Age Simulation of a Reservoir in Central Mexico
By Eric Gutierrez
National Water Commission, México

Valsequillo reservoir is located in the central part of México, (18°54'58"N 98°10'55"W); it is found at 2000 meters above the sea level. The reservoir is fed regularly by the rivers Atoyac and Alseseca with a maximum inflow of 16 m³/s. A three dimensional model (ELCOM) was implemented to learn about the hydrodynamics of the reservoir. There were two field campaigns to obtain the input data for the model. With a bathymetry of 80 meters resolution the hydrodynamic was simulated using the wind and temperature of the lake as the main forcing elements. The model gave good results reproducing the density and temperature distributions. However, the measure of velocity on the reservoir was so small that was difficult to reproduce. The results of residence time and water age agreed well with the historical data of the Water Commission management of the reservoir.

Tuesday, July 22, 2014 - 4:30pm-6:00pm

A New Locally Conservative Lagrangian-Eulerian Method for Hyperbolic Conservation and Balance Laws
By John Alexander Pérez Sepúlveda
ITM Institución Universitaria

In this work we make use of a locally conservative space-time finite volume approach in a Lagrangian-Eulerian framework, first developed in the context of parabolic convection-diffusion equations [1,2], to design a locally conservative scheme for balance laws, in order to account for the balance between numerical approximations of the hyperbolic flux function and the source term linked to steady solutions [3,4]. Our Lagrangian-Eulerian scheme is aimed to be independent of a particular structure of the source term [5]. The designed scheme is Riemann-solver-free, but if Riemann solutions are available for a particular problem at hand, it is somewhat natural to incorporate such information into the procedure, thus yielding flexibility for the development of distinct numerical strategies upon the specific model under consideration. A representative set of numerical experiments for nonlinear problems highly cited in the literature [5] - scalar and system - of hyperbolic conservation law and balance law types, are presented to illustrate the performance of the new method. We compare our numerical results with accurate approximate solutions or exact solutions whenever possible.

Control Philosophy of a Double Feed Asynchronous Machine for Power Optimization
By Patricia Sánchez
Universidad Central de Venezuela

In Eolic generation, double feed induction is highly used because it allows obtaining stable parameters through control of rotative currents vector. Therefore, it is necessary to maintain a trustworthy control. The objective of this research is to establish a control philosophy that allows operating the system for maximum efficiency of the turbine, considering the reactive power delivered to the grid in such a manner that it can cover its requirements in real time. The operation of the induction machine feed in the rotor, the behavior of the inverter, and the rectifier, was studied. We found that it is ideal to control the rectifier and the inverter associated to the rotor independently. An associated control that is convenient and simple was proposed according to the current and the complexity of the desired output. Simulation was carried out to test the proper operation of the system.

On the Mean Extinction-Time Estimate for Stochastic Population Models
By Fernando Vadillo
University of the Basque Country

The research on interacting population models has long been and will continue to be one of the dominant subjects in mathematical ecology; moreover, the persistence and extinction of these models is one of the most interesting and important topics, because it provides insight into their behavior. The mean extinction-time depends on the initial population size and satisfies the backward Kolmogorov differential equation, a linear second-order partial differential equation with variable coefficients; hence, finding analytical solutions poses severe problems, except in a few simple cases, so we can only compute numerical approximations. We study a classic Lotka-Volterra model using the backward Kolmogorov equation, and we have extended those ideas to a SIS epidemic model.

Numerical Simulations of Time-Dependent PDEs
By Fernando Vadillo
University of the Basque Country

When a time-dependent partial differential equation (PDE) is discretized in space with a spectral method, the result is a coupled system of ordinary differential equations (ODEs) in time. This is the notion of the *method of lines* (MOL) and the resulting set of ODEs is stiff; the stiffness problem may be even exacerbated sometimes. The linear terms are primarily responsible for the stiffness, with rapid exponential decay of some modes (as in a dissipative PDE), or a rapid oscillation of some modes (as in a dispersive PDE). Therefore, for a time-dependent PDE which combines low-order nonlinear terms with higher-order linear terms, it is desirable to use higher-order approximation in space and time.

In our researches, we develop numerical methods for time-dependent PDEs using different techniques: an exponential time differencing method in 2008, an integrating factor in 2010, and differentiation matrices in the theoretical frame of matrix differential equations in 2012 and 2013.

A Mathematical and Computational Study for Hyperbolic Conservation Laws with Stiff Source Terms
By Abel Alvarez Bustos
University of Campinas

In this work, we are interested in the study of wave formation in a long time behaviour that appears in hyperbolic conservation laws with stiff, relaxing source terms, by means of numerical analysis and analytical approximations. Indeed, we developed a locally conservative unsplitting finite volume scheme by construction, with efficiency of the implementation and very low memory storage requirements. We obtained the analytical

approximation in two steps. Firstly, we apply a mollification approach as an effective method of regularization for solving an ill-posed problem associated to a 3x3 Euler system as a model problem with relaxation source term. Secondly, using this method, we reduced the Euler system to a 2x2 system of balance law, which in turn was solved by using the method of characteristics [1,2]. The scheme is also used to reproduce consistent solutions for the more general Euler equations with gravity and friction, recently published in the specialized literature [3,4,5].

GUI Development for Pre-Processing Data and its Coupling with a Tsunami Numerical Model

By Adriana Liendo Sánchez

Venezuelan Foundation for Seismological Research

Geological events from seismogenic origin that occur in the ocean floor have the ability to generate tsunamis. To study these events numerical models that solve the shallow water equations integrated into the vertical have been developed. They allow the estimation of the maximum heights of waves and their arrival times to the coast. To this end, the CICESE used the model supported by UNESCO Goto, Ogawa adapting some necessary tools from the Matlab software to do the pre-processing of the data used for the representation of bathymetry and topography of the study region, as well as the representation of the marine surface deformation that generates a Tsunami theoretically. However, the reuse of these preprocessing tools tends to be complex and user error prone. For this reason, a graphical interface has been developed, adapting the original code so that it allows automatic interaction between the different modules that are used for simulation, based on a Wizard. It includes the bathymetry and topography interpolation based on a Python algorithm, automating part of the original processing. This interface significantly reduces the time intervention by the user, as well as any errors that a user could make during the preparation of the data manually. By using the GUI, the time spent by the user to run the simulation can be reduced up to 80%. The goal of this tool is to contribute to the assessment of potential tsunami scenarios for the Caribbean region, facilitating the simulation processes to be performed by users.

Computational Methods for Identification of Clusters in Petrographic Data

By Camila Martins Saporetti

Federal University of Juiz de Fora

The study of hydrocarbon reservoirs is crucial to define the characterization, productivity potential and the commercial prospects of an oil and gas field. A rock is considered a good reservoir if it has a considerable extent that identify a good porosity, an appreciable permeability and a good recovery efficiency.

The sedimentary petrofacies are a set of characteristics that individualize a particular group of rocks, and their

determination allows the inference of the heterogeneity of the reservoir. The conventional process in identifying petrofacies is performed by a geologist/petrologist in a manual manner. Thus, as the amount of data grows, the procedure becomes long and susceptible to failures. In this context, an automation of the tasks can improve the interpretation of the data and optimize the human resources. The techniques of Data Mining and Pattern Recognition becomes interesting to assist in the prediction of the characterization of a hydrocarbon reservoir.

This work aims to present a computational method based on clusters models developed to determine petrofacies amount in sedimentary thin-sections.

The proposed methodology is divided into Intra-well and Inter-well analysis. A Intra-well analysis involves the use of the Principal Component Analysis (PCA), clustering methods and validation criteria techniques.

In the Intra-well analysis, each cluster consists of thin sections with similar petrological characteristics, and suggests to the geologist/petrologist an idea of the petrofacies' formation. Different approaches for clustering were used, and the algorithmic parameters were adjusted by a process of exhaustive search, to maximize the measure of performance that reflects the quality of clusters.

In the Inter-well analysis, each predicted cluster in the Intra-well step is represented by the mean of its constituents and this information is used to build a graphical information which is returned to the geologist.

The data analyzed are thin section removed from exploration wells member Tibagy, Devonian of the Paraná Sedimentary Basin. The methodology gives a clear view of the data, which facilitates the interpretation of the clusters obtained.

Thus the computational method offers time-saving for the geologist/petrologist in the individualization of petrofacies, once the analysis produced is similar to those obtained by the conventional method of individualization.

Partial Differential Equations as Three-Dimensional Inverse Moment Problems

By Maria Beatriz Pintarelli

Universidad Nacional de La Plata

We consider partial differential equations of second order, for example the Klein-Gordon equation, the Poisson equation, on a region $E=(a_1,b_1)\times(a_2,b_2)\times(a_3,b_3)$. We will see that with a common procedure in all cases, we can write the equation in partial derivatives as a Fredholm integral equation of first kind and will solve this latter with the techniques of inverse problem moments. We will find an approximated solution and bounds for the error of the estimated solution using the techniques on problem of moments.

Workshop #1

Computational Mathematics in the Oil and Gas Industry

Organizer: German Larrazabal

Jaguar Exploration, Inc.

The oil and gas industry are a perfect target for applications of mathematical techniques. From subsurface exploration to production, refining, transport and finally distribution of oil, gas and products, real life mathematical and decision problems arise continuously. This mini-workshop aims at bringing together scientist and engineers from academia, research laboratories, and industry, to promote the application of mathematical techniques to the oil and gas industry problems. Papers on all aspects of mathematical theory, and computational and applied mathematics focused to solve oil and gas industry problems are invited to be presented at the mini-workshop.

Part I

Wednesday, July 23, 2014 - 9:30am-10:00am, 24G1

BSIT: An HPC Environment for Exploration

Geophysics

By Jose M. Cela

Barcelona Supercomputing Center

We introduce the BSIT environment that is able to perform different geophysical tasks, (forward modeling, RTM and full wave-form inversion), with different types of waves, (acoustic, elastic, viscoelastic and electromagnetic), over different architectures (symmetric multicores, GPUs, Xeon Phi). We describe the set of algorithmic approaches and the obtained performance.

Wednesday, July 23, 2014 - 10:30am-11:00am, 24G1

Randomized Linear Algebra in Large Scale Wave Propagation Simulation

By Victor Pereyra

Stanford University

We discuss the use of randomized linear algebra algorithms for problems in which the data does not fit in fast memory. For instance, when attempting to use Model Order Reduction for the 3D wave equation many simulations that arise in QC, survey planning and imaging, very large matrices occur. Monte Carlo methods can be applied for numerical rank calculations, least squares and the matrix multiplications required.

Wednesday, July 23, 2014 - 11:00am-11:30am, 24G1

The Mathematics of Seismic Reflection

By Miguel Dumett

San Diego State University

Generating a subsurface image is one of the goals of Seismic Reflection. Acoustic and elastic wave equations are the mathematical models utilized by seismic reflection. For that purpose, two-way time seismic data is acquired and cleaned of coherent and random noise. The different parameters of the model in the region of interest are unknown. Therefore, the mathematical approach is by inverse problem techniques. However, the size of the problem (thousands of square kms), the anisotropy aspect of the physics involved, etc., do not allow to solve the inverse problem straightforwardly. Fortunately, geophysicists have developed a sequence of tasks that allow, step by step, the construction of wave velocity models and by utilizing these models, finding a solution to the inverse problem is facilitated. The collection of applied mathematical techniques includes among others velocity analysis, NMO correction, stacking, migration and tomography. This talk aims to show some of the mathematics behind these techniques.

Part II

Wednesday, July 23, 2014 - 11:30am-12:00pm, 24G1

***Calculating the Probability of Geological Success
Prospects: A Critical Review***

By Rober Yibirin

Pacific Rubiales Energy

Over the past thirty years, the oil and gas industry has adopted several techniques to assess exploration prospects. Examples include probabilistic techniques, as well as techniques for decision-making under uncertainty. Concepts such as utility function, estimating expected values through Monte Carlo simulations, and probability of success, are common terms in exploration processes being implemented in many oil companies, regardless of their market size. We present a critical review of the concept of geologic risk, as it is currently applied in the oil and gas industry. Specifically, we try to estimate the probability of success of an exploration prospect in the context of decision-making under uncertainty. In the authors' opinion, a thorough review of the standard techniques used in the industry is needed. We suggest emphasizing those techniques related to the estimation of probabilities from the point of view of success-oriented domains. This will make a difference from other industries (aerospace, nuclear, and civil engineering, for example), in where similar reviews from the perspective of fault-oriented domain are presented.

Wednesday, July 23, 2014 - 2:00pm-2:30pm, 22G1

Reduced-Order Modeling Using Wavelet Transforms

By Miguel Argaez

It is well known that model-reduction methods borrow techniques typically found in data compression and current state-of-the-art techniques for data compression are based on the wavelet transforms. Given these facts, it is surprising that model reduction using wavelets has not received much attention and has not been adequately addressed in the literature. In this work, we propose a novel method for model reduction using wavelets. Specifically, we introduce techniques for deriving wavelet-based reduced-order models for solving inverse problems. To evaluate the performance of the wavelet-based reduced-order models, we conducted experiments on a set of linear and nonlinear partial differential equations, coming from heat-transfer and shock waves problems. The numerical results are then compared to model reduction based on the proper orthogonal decomposition (POD), which relies on a singular value decomposition (SVD) stage, and snapshots collection from the full-order model (FOM) discretization.

Wednesday, July 23, 2014 - 2:30pm-3:00pm, 22G1

***Uncertainty, Entropy, and Information Value in
Exploratory Projects***

By Rober Yibirin

Pacific Rubiales Energy

Value of information (VOI) techniques have wide use in the advanced stage of the hydrocarbon extraction business cycle. Yet, even though the early stage of the exploration process is critical (due to the nature of the decisions on acquisition data, as well as their relatively elevated cost), the industry considers that VOI techniques have a limited applicability on this stage. The reasons for this are, first, the comprehensive gap between the costs associated with this phase including exploratory drilling, and the monetary return for discovery. A second reason is the difficulty in solving some of the problems of data collection based on a decision under uncertainty. An alternative to using the VOI in the conditions under which your application is impractical, is to measure the reduction of uncertainty that can produce each study or data collection method. Based on this, it is possible to quantitatively estimate the reduction of uncertainty caused by the application of a study or method of estimating the entropy reduction in value (expected) that the method produces. This reduction in entropy can measure the difference between a priori entropy (uncertainty at the beginning of the experiment) and Media Conditional Entropy of the random variable. In this paper we evaluate and discuss the use of the concepts of uncertainty and value of information, the relationship between them and their use in the early stages of the Exploratory Process.

Part III

Wednesday, July 23, 2014 - 3:00pm-3:30pm, 22G1

Structural and Geometric Attributes in Seismic Interpretation

By German Larrazabal
Jaguar Exploration, Inc.

3D post-stack seismic data conditioning for a specific interpretation task requires removing the undesired and unnecessary, while improving the representation and interpretability of those parts of the information that are truly useful and valuable. A task that requires special attention for a better interpretation is the structural and geometric interpretation. In this talk, we show the mathematics behind the structural oriented attributes based on gradient structure tensor and a special geometric attributes such as volumetric curvature.

Wednesday, July 23, 2014 - 3:30pm-4:00pm, 22G1

FETKIN: Coupling Kinematic Restorations and Temperature to Predict Thrusting, Exhumation Histories, and Thermochronometric Ages

By Michael Raghieb
Ecopetrol - Instituto Colombiano del Petróleo

FETKIN is a C++ program for forward modeling thermochronological ages on a two-dimensional geological cross section. Modeled ages for various thermochronometers are computed from time-temperature histories that result from coupling the modeled kinematics of deformation obtained from commercial software for balanced reconstructions (2DMove) and a Finite Element (FEM) computation of temperatures. Additional capabilities include the ability to accommodate: a) A smooth change of topological relief; b) The influence of variation in rock physical properties; and c) Multi-kinetic modeling of fission-track ages and length distributions, as well as apatite and zircon (U-Th)/He, and muscovite $^{40}\text{Ar}/^{39}\text{Ar}$ systems. A joint first order analysis of the impact of erosion parameters and material properties improves age predictions and allows for a more complete analysis of observed cooling ages based on their modeled thermal histories. Thus, this paper presents a new software tool that has been developed as a basic support for the methodological approach used to build the kinematic restorations shown in this volume, which are the basic input for petroleum systems modelling and prediction in the Colombian Eastern Cordillera and Llanos foothills basin.

Wednesday, July 23, 2014 - 4:30pm-5:00pm, 22G1

Sparse Regularization for Data Mining and Approximation

By Reinaldo Sanchez
University of Texas at El Paso

Several natural signals are sparse or compressible in the sense that they have short representations when expressed in a suitable basis. We apply the selective nature of sparse representation to pattern recognition and dimensionality reduction problems. In this work, we present a sparse regularization optimization method, and study how sparse representation can be used to solve problems coming from classification of seismic events and restoration of seismic data with missing traces. We also discuss the effects of imposing group sparse representation, where the method is adjusted to generate solutions that are sparse at the group and individual feature levels, allowing an automatic feature extraction process.