

International Symposium on Mathematical Modeling 2016 (ISMM2016)

December 7–9, Casa Galván

The ISMM2016 is organized by the *Research Group on Numerical Analysis and Mathematical Modeling* from Universidad Autónoma Metropolitana, campus Iztapalapa. The main intention of this symposium is to bring together researchers and specialists from Mexico and abroad, who are interested in mathematics, modeling, numerical computing and applications, in order to increase our national and international networking as well as to promote research collaboration. We also want to promote student participation. Emphasis will be on control, inverse problems, dynamical systems and modeling with partial differential equations, focusing on new perspectives and methods to solve real problems.

Program. This meeting will take place at Casa Galván in Mexico City and will consist of six plenary lectures, thirteen invited talks and an open number of contributed posters. All these activities will be scheduled in an only one session from December 7 to 9, 2016.

Registration. Mrs. Beatriz Arce will be in charge of the registration desk. You will recognize her easily by the badge of the Symposium. She will register you and give you the event package. There is not fee for registration.

Lunch. Lunch will be offered for all the participants from 13:30 to 15:00 hours at Casa Galván on Wednesday and Thursday only. There are plenty nice places to have lunch on Friday.

Sponsors. Research Group on Numerical Analysis and Mathematical Modeling (2015 Research Award) and Department of Mathematics UAM-Iztapalapa.

Scientific and Organizing Committee. María Luisa Sandoval, Joaquín Delgado, Héctor Juárez and Héctor Morales.

SCHEDULE

	WEDNESDAY 7	THURSDAY 8	FRIDAY 9
9:00-9:20	REGISTRATION		
9:20-10:00	OPENING	JUÁREZ-VALENCIA	DELGADO-FERNÁNDEZ
10:00-11:00	KNOBLOCH	SHIMA	VELASCO-BELMONT
11:00-11:20	COFFEE	COFFEE	COFFEE
11:20-12:00	DOMÍNGUEZ-MOTA	CAPISTRAN-OCAMPO	GONZÁLEZ-CASANOVA
12:00-12:40	MORELES-VÁZQUEZ	DIAZ-VIERA	RIOS-SOLÍS
12:40-13:20	CORONADO-GALLARDO	ITURRARARÁN-VIVEROS	SANDOVAL-SOLÍS
13:20-15:00	LUNCH	LUNCH	LUNCH
15:00-16:00	DE LOS REYES	FENTON	BRANDÁN-SIQUÉS
16:00-16:40	POSTER & COFFEE	POSTER & COFFEE	POSTER & COFFEE
16:40-17:20	LÓPEZ-LÓPEZ	HERNÁNDEZ-DUEÑAS	PANEL: TRENDING TOPICS IN MODELING
17:20-18:00			CLOSING

INTERNATIONAL SYMPOSIUM ON MATHEMATICAL MODELING 2016

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<http://mat.izt.uam.mx/mat/index.php/eventos-2016/ismm-2016>

ABSTRACTS

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Posters: pages 13 to 20

PLENARY SPEAKERS

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CONTRAST-ENHANCED DIGITAL MAMMOGRAPHY IMAGES: CONVENTIONAL AND TEXTURE DESCRIPTOR ANALYSES

Contrast-enhanced digital mammography (CEDM) is a radiological technique based on the subtraction of images of the breast after an iodinated contrast-medium (CM) injection. We present results of a clinical study of CEDM images of 18 patients (cancer and benign) acquired 1 to 5 minutes after CM injection. Firstly, CEDM images of the adipose, glandular tissue and lesion regions-of-interest (ROIs) were correlated (via their mean pixel value) with blood and lymphatic microvascular density; secondly, texture descriptors were defined and evaluated at the ROIs and further analyzed in terms of a logistic regression. A linear combination of two texture descriptors discriminated between malignant and benign lesion with 79% specificity and 93% sensitivity. Results will be discussed.

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BI-LEVEL OPTIMIZATION APPROACHES FOR LEARNING THE NOISE
MODEL IN VARIATIONAL IMAGE PROCESSING

In order to determine the noise model in corrupted images, we propose a bilevel optimization approach in function space with the variational image restoration models as constraints. In the flavour of supervised machine learning, the approach presupposes the existence of a training set of clean and noisy images. The problems are treated as mathematical programs with variational inequality constraints and tailored regularization schemes for the approximation of the optimal parameters are proposed. Instead of relying on a priori statistical assumptions on the training set, the optimal parameter values are numerically computed by using a dynamically sampled quasi-Newton method, together with semismooth Newton algorithms for the solution of the image restoration subproblems.

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MATHEMATICAL MODELING OF CARDIAC ARRHYTHMIAS; HOW CLOSE
ARE WE TO THE REAL THING?

Heart modeling is a challenging problem because of the complex emerging behavior going from single cell to tissue. In this talk, we will discuss how we use a combined experimental, numerical and theoretical approach to better understand the dynamics of cardiac arrhythmias. We will show how heart dynamics is modeled and how large scale GPU simulations are used to better understand cardiac arrhythmias and to develop novel methods to control and terminate arrhythmias

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SOLIDIFICATION FRONTS IN SUPERCOOLED LIQUIDS: HOW RAPID
FRONTS CAN LEAD TO DISORDERED GLASSY SOLIDS

Using dynamical density functional theory we calculate the speed of solidification fronts advancing into a quenched two-dimensional model fluid of soft-core particles. We find that solidification fronts can advance via two different mechanisms, depending on the depth of the quench. For shallow quenches, the front propagation is via a nonlinear mechanism. For deep quenches, front propagation is governed by a linear mechanism and in this regime the front speed is determined via a marginal stability analysis. We find that the density modulations generated behind the advancing front have a characteristic scale that differs from the wavelength of the density modulation in thermodynamic equilibrium, i.e., the spacing between the crystal planes in the equilibrium crystal. This leads to the subsequent development of disorder in the solids that are formed. In a one-component fluid, the particles are able to rearrange to form a well-ordered crystal, with few defects. However, solidification fronts in a binary mixture exhibiting crystalline phases with square and hexagonal ordering generate solids that are unable to rearrange after the passage of the solidification front and a significant amount of disorder remains in the system.

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NUMERICAL STUDY OF SHALLOW MARITIME CLOUDS USING THE
SUPER-DROPLET METHOD

The Super-Droplet Method (SDM) is a particle-based and probabilistic scheme to simulate cloud microphysics [1]. This method can accurately simulate the time evolution of aerosol / cloud / precipitation particles with less demand on computation. Recently, we have applied the SDM to two types of shallow maritime clouds, cumuli and stratocumuli. In this talk, some of the results will be presented after introducing the method briefly. [1] S. Shima et al., Q. J. R. Meteorol. Soc. 135, 1307-1320 (2009).doi:10.1002/qj.441

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MULTI-CLASS TRAFFIC MODELS

The kinetic theory approach to study traffic problems has been followed to understand the dynamical behavior for vehicles in a highway. In the literature, some phenomena present in the empirical data have been described according to the so called Kerner's three phases theory. It identifies the free (F), synchronized (S) and the wide moving jam (W) as the phases of traffic, going from the free to the congested states. The synchronized and the wide moving jam phases correspond to the congested situation. Though the phases F and W have been modeled with macroscopic models, the S phase has resisted to all attempts in the macroscopic point of view. In this talk we will present a kinetic based model to arrive to a synchronized phase in a macroscopic model for two classes of drivers. The main points to take account for an explanation, are given through the over-acceleration and adaptation effects along the highway.



HOME SPEAKERS

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POSTERIOR NUMERICAL ERROR CONTROL IN INVERSE PROBLEMS

This talk is on the Bayesian approach to inverse problems. I will describe a strategy to bound the numerical error in the construction of the posterior probability distribution. I will show examples using the Cauchy problem for scalar conservation laws

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MODELING FINES DETACHMENT AND THEIR EFFECT IN LOW SALINITY WATERFLOODING ON SANDSTONE CORE EXPERIMENTS

An attractive oil recovery process in sandstone reservoirs is the injection of low salinity water flooding. By this mean, the rock-fluid dynamic properties are modified and additional oil is recovered. A lateral effect of the low salinity is the detachment of fines, their further migration and possible clogging of porous throats. This phenomenon reduces the permeability and can cause undesired problems. In this work we develop a single-phase model to describe fines detachment from the rock due to the salinity reduction, their migration, the pore clogging and the effect on the permeability. The involved 3D partial differential equation set is solved by the finite element method. The model is applied to low salinity water flooding experiments in sandstone cores.

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TRAVELING WAVES AND BIFURCATION IN CONTINUOUS TRAFFIC FLOW

We present a survey of join work on the study of traveling waves of 1D continuous traffic flow models, its reduction to a dynamical system and the global map of the different type of codimension 2 bifurcations: Takens-Bogdanov, Hopf, Bautin, homoclinic. In the present status we are investigating the stability of traveling waves and the mechanism of instability that lead to spatial patterns.

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FLOW AND TRANSPORT MODEL IN POROUS MEDIA AT CORE SCALE USING A FINITE ELEMENT METHOD

In this work, a general flow and transport model in porous media to simulate, analyze and interpret enhanced oil recovery tests at core scale under laboratory conditions is presented. The flow model is a single phase slightly compressible, whereas, the multicomponent transport model includes physical-chemical phenomena such as advection, diffusion, dispersion, adsorption-desorption, and reactions. For the numerical solution is applied a finite element method and its computational implementation was carried out in Python using FeniCS project. From the methodological point of view, each stage of model development (conceptual, mathematical, numerical and computational) is described. The resulting coupled flow and transport model is numerically validated in a case study.

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NUMERICAL SIMULATION OF RAINWATER INFILTRATION USING FINITE
DIFFERENCES

In this talk, to analyze rainwater infiltration through a road structure, we present the results of a simulation carried out to produce numerical approximations to the solutions of Richards' equation using general finite differences. Some examples and benchmarks using finite element method show that this approach is suitable to describe infiltration accurately.

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CONTROL DISTRIBUIDO Y FUNCIONES DE BASE RADIAL.

En esta plática revisaremos cual es la situación actual de los métodos de funciones de base radial para la solución de problemas en EDP's de control distribuido. A partir de esta revisión, formularemos dos nuevos algoritmos de FBR para la solución de problemas parabólicos estacionarios de control distribuido. Discutiremos las limitaciones y alcances de estos métodos así como las perspectivas actuales en el área.

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TWO-LAYER SHALLOW WATER FLOWS IN CHANNELS

We present a central scheme for two-layer shallow water flows in channels of arbitrary geometry. Geometries where the cross sections consist of vertical walls of variable width will be considered, followed by general cross-sectional areas. Consideration of conservation, near steady-state accuracy and positivity near dry states will be discussed. Numerical results will be shown for a variety of unsteady and near steady flows. This is joint work with Jorge Balbás.

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INVERSION OF SEISMIC VELOCITIES COMBINING SELF-ORGANIZED
MAPS AND

We apply Self-Organizing maps to classify seismic reflection data into a set of three different facies. This gives us our starting velocity model. In order to test this initial layered velocity model, the elastodynamic response of the stack of plane-layers upon an incident plane wave is computed by means of the Thomson-Haskell method. We compare the synthetic response with the measured data. We perform an inversion using non-linear squares to fit the synthetic traces and the real data. We see that the final velocity model has a feasible structure and is correlated with the seismic.

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THE CAUCHY PROBLEM ON IRREGULAR ANNULAR REGIONS: A
NUMERICAL APPROACH

In this talk we present a variational formulation to find stable solutions of the Cauchy problem for the Laplace equation in complex annular regions. This problem arises in many practical applications but it is ill-posed. We reformulate the problem as an optimal control problem where the control acts on the interior boundary of the annular domain. The solution of minimal norm is found with a methodology that combines an iterative conjugate gradient algorithm and finite element discretizations.

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STABILIZING A JOSEPHSON JUNCTION ARRAY MEMORY AROUND AN
UNSTABLE EQUILIBRIUM: A CONTROL APPROACH.

In this talk we use a model of three ordinary differential equations associated with a three Josephson Junctions Array Memory (JJAM) in order to

stabilize the system around an unstable equilibrium. To reach that goal we use optimal control techniques by defining a cost functional and calculating its differential via a perturbation analysis. For the computational solution of the optimal control problem we consider a conjugate gradient algorithm for quadratic functionals in Hilbert spaces.

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MODELS IN FRACTIONAL MECHANICS

In this talk we show a derivation of fractional differential equations in Continuum Mechanics and Electromagnetism. Fractional derivatives are introduced in generalized constitute equations. Our motivation comes from Curie's law (1989) in Capacitor Theory and Nutting's equation (1921). The latter relates stress and deformation in composite materials. Also we show some applications on Biomedicine and provide a response to a bioimpedance query.

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INVERSE PROBLEMS IN TRANSPORTATION SYSTEMS

This talk is about two different inverse problems that arise in transportation systems. The first inverse problem is about determining an Origin-Destination matrix: how to infer the amount of people going from one point of the city to the other when you only have some traffic counts in the network. The second problem is about the determination of a timetable for a bus company when you already have an assignment of the drivers and the vehicles to the trips. Both problems are tackled from the combinatorial optimization point of view.

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TRACER TESTS: MODELING AND NUMERICAL SIMULATION

Tracer tests in oil reservoirs are aimed at diagnosing the presence of high permeability channels and characterizing subsurface formations in the vicinity of the well. They help to determine the porosity, dispersion coefficients and thickness of the production layer. This talk is about two different tracer tests problems. First, we present the numerical modeling of the injection phase in a cylindrical region with constant porosity for a single well push-pull test. The second problem studies the dynamics of tracers when tests are performed in a well with bipolar flow.



POSTER PRESENTATIONS

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SYMMETRIC HORSESHOE PERIODIC ORBITS WITH ZERO ANGULAR MOMENTUM ON THREE-BODY PROBLEM

We present some families of horseshoe periodic orbits in particular zero angular momentum on three-body problem. The considered system is a symmetric version of the one formed by Saturn, Janus and Epimetheus. We use a mass ratio equal, for this mass ratio the satellites have a significantly bigger influence on the planet than in the classical Saturn, Janus and Epimetheus system. To obtain periodic orbits, we search those horseshoe orbits passing through two reversible configurations. A particular kind of periodic orbits where the minor bodies follow the same path is discussed.

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MONTE CARLO ESTIMATION OF THE INTERNAL ABSORBED DOSE DISTRIBUTION IN A SOLID TUMOR USING TOMOGRAPHIC DATA

In this work we developed a methodology to estimate the internal absorbed dose distribution in a solid tumor at the voxel level, which is of interest in the dosimetry of targeted radionuclide therapies. The methodology involves computing a dose voxel kernel for the radionuclide of interest using a code for the Monte Carlo simulation of radiation transport, in our case EGSnrc. This kernel is convolved with a cumulated activity distribution resulting from quantified SPECT/CT studies to obtain the absorbed dose distribution. Operations involved include image registration, region selection, kinetic modeling and integration of time-activity curves. A software named xgrid3d was developed to address these in a user-friendly manner.

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MODELS AND ALGORITHMS TO ESTIMATE ORIGIN-DESTINATION
MATRICES

Estimate or adjust an origin-destination (O-D) demand matrix from a relatively small amount of observed data, have become an important issue for public transport engineering due to the cost and effort involved in obtaining such matrices from surveys. Among the data that can be used in the process of estimation, the flow of passengers in some segments of the network is one of those data that can be obtained relatively easy. So, given an obsolete (O-D) demand matrix, it is desired to update it to a near state such that, after a performance of a transit equilibrium assignment, the resulting flows in the segments are as similar as possible to the observed flows. In this work we explore different methodologies to solve the problem of estimate an O-D demand matrix and compare each others performance in three different transit networks: one small (hypothetic), one medium-sized (Winnipeg City) and one large-sized (Mexico City and Metropolitan area)

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DEGENERATE BOGDANOV-TAKENS BIFURCATIONS AND TURING
INSTABILITY ON A BAZYKIN MODEL

The Bazykin model is a two-dimensional predator-prey dynamical system of codim 3. Alexander D. Bazykin conjectured that the system can exhibits a degenerate Bogdanov-Takens bifuraction and Yuri A. Kuznetsov proved it and give how to calculate the normal forms. We calculate numerically the bifurcation diagram and the normal form of the model. On the other hand, we study the Turing instability adding diffusion to the system.

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NUMERICAL SOLUTION OF THE
NAVIER-STOKES-POISSON-NERNST-PLANCK EQUATIONS FOR
ELECTROKINETIC FLOW

Recent development in micro/nano-technologies have stimulated research interest towards the design, fabrication and implementation of micro/nano-fluidic devices due to its increasingly important applications in electrochemistry, environmental technologies, alternative energy sources, biotechnology, biomedical engineering and MEMS, among many others.

An important non-mechanical actuating technique for micro/nano-fluidics that has been used for the development of micro/nano-devices is employing electrokinetic flow, which is one of the most typical multiphysical transport phenomena. The electrokinetic flow involves multiple processes including fluid flow, ionic diffusion, electrostatic interaction and sometimes energy transfer.

The theory for electrokinetic flow is built up from the study of fluid dynamics in microchannels (Navier-Stokes equations) and electrodiffusion (Poisson-Nernst-Planck equations), obtaining a system of strongly coupled nonlinear differential equations modeling flow dissolved in an electrolyte under the action of internal and external electric fields.

In this poster, will be presented the numerical solutions of the Navier-Stokes-Poisson-Nernst-Planck equations for electrokinetic flow in two dimensions. These numerical solutions were obtained from an iterative algorithm using the projection method and finite element method.

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GLOBAL BIFURCATION MAP OF HOMOGENEOUS STATES IN GRAY SCOTT
MODEL

We study spatially homogeneous states of the system of reaction-diffusion of Gray-Scott of an autocatalytic reaction in dimension 2. The resulting

dynamical system depending on two parameters has a rich structure of bifurcations. We give a rigorous proof on the existence of Takens-Bogdanov and Bautin bifurcations. The global extension of the local curves of Hopf and homoclinic curves obtained numerically is presented together with the phase portraits. A study of Turing instabilities is in progress.

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MODELING 2-D WAVE PROPAGATION IN POROELASTIC MEDIA USING LOCALLY ONE-DIMENSION (LOD) IMPLICIT FINITE DIFFERENCES

We develop a locally one-dimension (LOD) implicit finite-difference scheme to model wave propagation in 2-D poroelastic media. Since the method is implicit in time we must solve a set of two linear systems of equations per time step, with the advantage that these systems are tridiagonal and are solved through Thomas' algorithm. The greatest benefit of time implicit schemes is the unconditional stability. In practice, this implies that one can be able to use time steps Δt of one order of magnitude (or even more) larger than that of explicit schemes, with the inherent computational cost reduction. We present a numerical implementation of the Biot's equations for 2-D problems based upon the LOD implicit finite differences that clearly illustrates the existence of the fast and slow P-waves, one of the fundamental results of Biot's theory.

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NULL CONTROLLABILITY OF A DIFFUSION PROCESSES ON A SPHERE IN \mathbb{R}^3

The main goal of this work is to study computationally the null controllability of a diffusion process on the surface of a sphere in \mathbb{R}^3 . To achieve this goal, we employ a methodology combining finite differences for the time discretization, finite elements for the space approximation, and a conjugate gradient algorithm for the iterative solution of the discrete control problem.

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MODELING FINES DETACHMENT AND MIGRATION INDUCED BY LOW
SALINITY WATER INJECTION IN OIL RESERVOIRS.

In the oil industry one of the central points is the development of new techniques for the better oil recovery process, one of them consists in clogging of porous throats in an oil reservoir through the clogging of fines (very small pieces of a rock).

When injecting of low salinity water to the rock, small sandstones are detached (fines adhered) and travel in the water (fines mobile) until they possibly clog the pores throats (fines clogging). In this work we present the modeling of the detachment, migration and pore clogging by fines in a two-phase flow: water and oil. For this, a system involving eight partial differential equations (PDE) is proposed, which are: four equations for the two-phase flow, one for the salt concentration and three equations for the fines concentration. These equations are commonly coupled through the permeability. If we consider the constant permeability the PDE system is decoupled, this allows to resolve the two-phase flow regardless of the concentrations.

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BAYESIAN PARAMETER ESTIMATION IN PHARMACOKINETICS MODELS

The pharmaceutical industry is always looking for new ways that help the development process of new compounds to be more efficient. According to the Food and Drug Administration of the United States, simulation and mathematical and computational modeling are useful instruments that improve the effectiveness in the safe and efficient elaboration of new drugs.

In this work, the applied methodology consist in modeling the drug concentration evolution in a certain organism using a system of ordinary differential equations; this kind of models, which are based on biological and pharmacological principles, are known as pharmacokinetics models. The pa-

parameter distributions of each model will be estimated employing Bayesian inference, specifically through Markov Chain Monte Carlo methods.

In particular, two examples will exemplify this technique. Firstly, with the kinetics of theophylline in humans, a compound used in the treatment of certain respiratory alignments; secondly, with the concentration in time of the encapsulated-liposome cisplatin administered to mice, a chemotherapy agent.

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RAYLEIGH-BÉNARD CONVECTION IN A OPEN CUBE AND
PARALLELLIPEDIC CONTAINER WITH ADIABATIC SIDE WALLS

We consider a viscous fluid heated from below in a parallelepipedic container for different height-base ratios and an open surface. The equations are Boussinesq approximation with Rayleigh and Prandtl numbers as parameters. We use Galerkin method to compute the first bifurcation values for deviations from a stationary state in the linear approximation. Our results compare well with known values of parallelepipedic closed containers in the literature, after a symmetry argument is involved.

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FINITE VOLUME METHODS IN SHALLOW WATER 1-D

The shallow water equations are nonlinear hyperbolic equations and usually numerical methods are needed to find solutions. Also, these equations may develop discontinuous solution even if the initial data is continuous, so special numerical techniques must be designed to capture this phenomenon. Finite volume methods, and in particular Godunov schemes, have shown to be a good option in such cases. In this work we present the solutions obtained with different schemes when the topography is flat and also when it is not flat.

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NUMERICAL SOLUTION OF 1D SHALLOW WATER EQUATIONS IN
RECTANGULAR CHANNELS USING DISCONTINUOUS GALERKIN METHOD

The one-dimensional shallow water equations are formed by a non-linear hyperbolic system of equations that describes depth and flow of water in an open channel. On the other hand, the discontinuous Galerkin (DG) method is a numerical scheme that helps to find an approximation to the solution of a system of differential equations. In addition, it can be seen as a combination of finite element (FE) and finite volume (FV) methods. Because it uses the same shape functions as in the FE method, but it imposes the numerical flows developed in the FV method as boundary conditions in each element. Numerical schemes that decreases total variation are applied to avoid spurious oscillations in the solution as time progresses: The TVD-Euler forward and TVD second order Runge-Kutta methods. However, these methods have problems in vicinity of discontinuities or steep slopes. Slope limiters are used to deal with them. We only present the minmod limiter applied after every intermediate step of the TVD Runge-Kutta method since it provides better results. Finally, the numerical fluxes used in this work are: HLL flux, Lax-Friedrichs flux and Roe flux. The former has shown the best results. We present numerical solution for one dimensional shallow water equations with DG method. Numerical tests included : flow over a bump, flow over an irregular bed and flow over a bowl. We also show the numerical results with the slope limiter applied to either the water depth or the water surface.

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AN APPLICATION OF THE HEDONIC PRICING MODEL TO THE HOUSING
MARKET IN ACAPULCO

In this work we test through the application of the Hedonic Pricing Method that the distance of a housing in Acapulco to one of the most insecure zones in this city is significant for the determination of housing pricing

in the market. Our model relates the price of housing with other variables like level of public services, physical characteristics, among other variables. We find that the effect on the price is negative, namely as the housing are closer to this zone the value of housing depreciate .

