Poster Session

Calculating the width parameter of the potential energy surface of some chemical reactions using simple quantum mechanics

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A simple computational procedure is used for defining the width parameter of the potential energy surface of different elementary interchange chemical reactions.

Concerning the computational theoretical basis, a simplified quantum mechanical treatment is presented for the phenomena of the reactive scattering of an atom A and a diatomic molecule BC giving rise to a free atom C together with a diatomic molecule AB.

The mathematical formula derived allows the reduced masses to vary smoothly with the reaction coordinate "u". This property is extremely important, since it is the actual nature in which the reduced masses of reactants change into those of the products.

Also the treatment under consideration uses Eckhart potential , which truly and completely describes the reaction process . This potential allows the reactants to start at the initial state asymptote $-\infty$, with a certain initial potential energy $v_{-\infty}$, ascending smoothly over a definite potential barrier, descending again smoothly, and finally ending with a certain constant final potential level $v_{+\infty}$ at the far final state asymptote $+\infty$.

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Classical Hybrid Monte-Carlo Simulation of the Interconversion of Hexabromocyclododecane stereoisomers

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The interconversion of the six main stereoisomers of the flame retardant hexabromocyclododecane (HBCD) is investigated by means of statistical thermodynamics using classical force-fields. (+-)-alpha-, (+-)-beta- and (+-)-gamma-HBCD interconvert by swapping of absolute configurations on the three different (BrHC ??? CHBr)-moieties. The approach avoids saddle-point energy computations, but relies on classical thermodynamic simulation and pursues three consecutive steps. First, the application of classical hybrid Monte-Carlo simulations for quantum mechanical processes is justified. Second, the problem of insufficient convergence properties of hybrid Monte-Carlo methods for the generation of low temperature canonical ensembles is solved by an interpolation approach. Third, it is shown how free energy differences among stereoisomers are derived and how they can be used for the computation of interconversion rates. The simulation results confirm the experimentally observed interconversion rates and correctly identify alpha-HBCD as a thermodynamical sink in the oscillating mixture of stereoisomers.

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A heuristic mathematical model for the core circadian clock in Neurospora crassa.

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Circadian rhythms are cycles of about 24 hours, which provide temporal information to various biological processes such as sleep/wake cycle. These rhythms have been observed in many organisms from cyanobacteria up to humans. The molecular mechanisms of circadian rhythms are similar from Neurospora crassa to mammals. Therefore, a comprehensive analysis of its circadian rhythm will facilitate our understanding of the underlying properties of the human circadian rhythms.The Neurospora circadian clock is a molecular mechanism consisting of complex gene regulations (activation, inhibition), post- transcriptional and post-translational regulations that create a time delayed negative feedback loop. An initial mathematical approach is presented to model the core of this clock. Parameter estimation, bifurcation and stability analysis is presented to determine the dynamical features of this mathematical model.

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Linear Volterra Stieltjes integral equations in the sense of the Perron integral and an application to functional differential equations

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We prove an existence result for linear Volterra Stieltjes integral equations with Perron-Stieltijes type integrals. As an application, we consider a linear functional differential equations perturbed by a Perron integrable function and we get and existence result for this equation.

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A Class of Solutions for the Generalized Langevin Equation Driven by Stable Processes

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Random motions of particles are generally modelled as diffusions driven by some noise process and solutions to the resulting stochastic differential equations are searched. When white noise is detected the Langevin equation may arise as a suitable model. On the other hand, in modelling a large variety of complex systems, one encounters anomalous diffusive phenomena. In this case, Generalized Langevin Equation (GLE) driven by stable processes with infinite variance might well be considered. Assuming stability index 1

A Reaction-Diffusion Model for Cell Populations in the Colonic Crypt

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The human colon contains microscopic finger-like invaginations called crypts that are responsible for continuous epithelial cell reproduction. Inside the crypt, stem cells accumulate near the base and migrate up the crypt walls while proliferating and differentiating, until finally exiting through the top of the crypt as a completely differentiated and non-proliferating cell. Once the crypt establishes a specific cell organization, it splits into two new crypts. In a cancerous colon, we see an abundance of stem cells throughout the entire crypt, which leads to abnormal crypt fission and eventually polyp-like adenoma. Our goal is to model the normal cell regulation inside the crypt using a reaction-diffusion model in a 2-D cylindrical domain, and then perturb the system to gain insight into how it becomes disorganized. We consider three cell populations: stem cells, proliferating cells, and differentiated cells. The non-linear reaction terms describe cell production, while the diffusion terms describe the migratory effect throughout the crypt.

Equilibrium in a two-oscillator system coupled to a chaotic environment

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This study explores the dynamics underlying the coupling of two oscillators to classical low-dimensional chaos. In particular, we examine the case in which the oscillators are close in frequency. It is shown that, given sufficient coupling, resonant oscillators can exchange energy and equilibrate to nonequipartition values. The off-resonant cases studied were shown to have equilibrium momentum distributions close to Gaussian. We found additionally that the Rugh and kinetic temperatures relaxed in time in a quite similar manner.

Predator-Prey Relationship in a Closed Habitat

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In this paper we study Predator-Prey dynamics by utilizing, as a basis for investigation, the Haefner-Holling Model of Prediction in Simple Communities. The interactivity and stability of a moose and wolf relationship will be analyzed mathematically. The general form of this model will be reviewed and applied to an environmental system that is represented by three sub-systems: the habitat, the moose population, and the wolf population. Looking at seven specific variables: moose reproduction rate, moose habitat carrying capacity, moose/wolf encounter rate, total time available for moose to forage, time required for wolf to harvest a moose, conversion rate of victims to new predators and per capita wolf death rate, predictions of future population stability will be examined. A look into a hypothetical situation will conclude the investigation to insure integrity of the model.

Effects of Optimal Antipredator Behavior of Prey on Predator-Prey Dynamics: The Role of Refuges

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The purpose of this paper is to give some mathematical analysis on the predator-prey models where prey has anti-predator behavior with the use of refuges. The models examined were introduced by Vlastimil Krivan in his paper, "Effects of Optimal Anti-predator Behavior of Prey on Predator-Prey Dynamics: The Role of Refuges", and were based on the Lotka-Volterra and Holling Type II functional responses. Analysis on local and global stability for equilibrium solutions will be performed on proposed values for given variables, and constraints for stability will be studied. We also demonstrate numerical simulation and discuss the ecological implications of our results.

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Sufficient Conditions for Optimality of Bang-bang Controls in Compartmental Models for Cancer Chemotherapy with Blocking Agents

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In mathematical models for cancer chemotherapy, cell-cycle specificity is an important aspect that allows for a more precise modeling of the actions of drugs. In this poster, a cell-cycle specific compartmental model for the growth of cancer cells that combines a cytotoxic (killing) agent with a cytostatic (blocking) agent is considered. The blocking agent is used to synchronize the transitions of the cell through the cell-cycle and thus leads to a more effective action of the killing agent. We analyze the model as an optimal control problem with the objective to minimize a weighted average of the cancer cells in the various compartments over a fixed therapy horizon, both over the course of therapy and at the end of the therapy horizon, while keeping the side effects of the drugs under control. For this model, candidates for optimal controls are bang-bang controls corresponding to full dose treatment intervals with rest periods in between. However, the optimality of these controls, particularly at the switching times, has to be verified. In this poster an algorithm will be formulated that allows us to verify the overall optimality of bang-bang trajectories.

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From Chaotic to Hyperchaotic Rossler model: Periodic Orbits analysis.

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An hyperchaotic dynamical system is defined by two positive Lyapunov exponents. This is only possible for at least a four dimensional system as for example the Rössler (1979) hyperchaotic model where $\dot{x} = -(y + z)$, $\dot{y} = x + ay + w$, $\dot{z} = b + xz$ and $\dot{w} = -cz + dw$ with a=0.25, b=3.0, c=0.5 and d=0.05. Unlike the well-known 3D chaotic model, this system has been barely studied. Applying our periodic orbits (POs) search strategy we found 2, 3, 5 and 10 POs of multiplicity one to four with a mean period of 6.5, 13.2, 19.9 and 26.7, respectively.To find them we have carried on a systematic search using the Stability Transformation (ST) method of Schmelcher and Diakonos (1997) combining with the Newton method. The combination of this two methods will improve the efficiency of the ST method since near the solution the Newton method converges quadratically. For the sake of completeness we have also studied the periodic orbits collection found in the traditional 3D Rössler model and we have investigated the differences between the chaotic and hyperchaotic Rössler systems.

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Bistable Fronts in Discrete Inhomogeneous Media

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Solution behavior of a bistable differential-difference equation with inhomogeneous diffusion is considered in depth. Employing a piece-wise linear nonlinearity, often referred to as McKean's caricature of the cubic, front solutions are constructed which correspond, in the case of homogeneous diffusion, to monotone traveling front solutions or stationary front solutions in the case of propagation failure. A general form for these fronts is given for essentially arbitrary inhomogeneous discrete diffusion, and conditions are given for the existence of solutions to the original discrete Nagumo equation. The specific case of one defect is considered in depth, giving a complete understanding of propagation failure and a grasp on changes in wave speed. Insight into the dynamic behavior of these front solutions as a function of the magnitude and relative position of the defects is obtained with the assistance of numerical results.

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Bifurcation and Stability Analysis of a Prey-Predator Aystem with a Reserved Area

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This paper analyzes a prey-predator system with a reserved area. The predator functional response is taken to be of Holling type II .It is assumed that the habitat is divided into two zones, namely free zone and the other is reserved zone where predation is prohibited. The local and global stability analysis have been carried out. When the carrying capacity of the environment crosses a critical value, we determine that strictly positive equilibrium enters into Hopf bifurcation. We obtain conditions which influence the persistence of all the populations. Numerical simulation with a hypothetical set of data has been done to support the analytical findings.

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Optimal Control for Multi-Drug Chemotherapies for Cell-Cycle Specific Models

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In mathematical models for cancer chemotherapy, cell-cycle specificity is an important aspect that allows for a more precise modeling of the actions of drugs. In this poster, a cell-cycle specific compartmental model for the growth of cancer cells that combines a cytotoxic (killing) agent with a recruiting agent is considered. This kind of therapy is particularly relevant for leukemia which is characterized by long s??jour times of the cancer cells in the dormant compartment. We analyze the model as an optimal control problem with the objective to minimize a weighted average of the cancer cells in the various compartments over a fixed therapy horizon, both over the course of therapy and at the end of the therapy horizon, while keeping the side effects of the drugs under control. The model will be considered without and with linear (one- or two-compartment) pharmacokinetic models on the drugs. The effect that the inclusion of these pharmacokinetic models has on the structure of solutions - optimal dosage protocols - will be analyzed. It is shown that in either case optimal controls are bang-bang and numerical examples of optimal solutions will be given.

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Analysis of a System of Differential Equations: Population and Harvesting Dynamics of the North Carolina Red Drum

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This paper focuses on the population and harvesting dynamics of the North Carolina Red Drum. The model used for analysis is a two dimensional nonlinear model. The purpose of this ODE model is to assess damage on the Red Drum stock size prior to year 2000, and to return the stock size to a healthy number but avoiding overpopulation. There are nine parameters used in this model. Some of the parameters were approximated using sensitivity analysis, while some were gathered using data from 1990. Three different cases were tested, using various parameters. It was found that in each case, there were two sets of real equilibrium points, although only one of them was asymptotically stable. This model has proved to be an efficient way to regulate fishing effort in North Carolina. In 2009, the state of North Carolina fisheries was taken out of the 'over fished' category and placed under the 'recovering' category.

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Recursiveness in impulsive semidynamical systems

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We consider a class of impulsive semidynamical systems and we study recursiveness properties for these systems. We present results which relate minimal sets, recurrent sets and almost periodic sets.

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Optical Biosensors with Arrays of Reacting Zones

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Optical biosensors are widely used for measuring reaction rate constants and for understanding surface-volume reaction dynamics. Early biosensors included a single reacting zone for the study of a single reaction. New devices include arrays of reacting zones in a single flow channel, allowing for the study of up to four hundred reactions at once. Real time measurements of bound reactants in a reacting zone are taken and averaged to obtain a sensogram of the bound state. We discuss a model for ligand depletion and bound state evolution over arrays of reacting zones and extend previous work to arrays of circular reacting zones and arrays having reacting zones with different association and dissociation rates. The effect of these extensions is quantified and compared with previous results.

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