WORKSHOP ON ANALYSIS AND ITS APPLICATIONS IN BIOLOGY AND PHYSIOLOGY

WORKSHOPS

CASTS

理論科學研究中心

Center for Advanced Study in Theoretical Sciences

2014. 12. 26-31

Langevin and Fokker-Planck Analyses of Inhibited Molecular Passing Processes in Nanoporous Materials

Prof. Chi-Jen Wang

Inhibited passing of reactant and product molecules within the linear pores of nanoporous catalytic materials strongly reduces reactivity. The dependence of the molecule passing propensity P on pore radius R is analyzed utilizing Langevin dynamics to account for solvent effects. We find that P~(Râˆ'Rc)^Ï*ƒ*, where no passing for Râ‰¤Rc, with Ï*ƒ* below the transition state theory value. The high-dimensional Fokker-Planck analysis facilitates an effective small-P approximation, and dimensional reduction enables utilization of conformal mapping ideas. We analyze passing for spherical molecules and also assess the effect of rotational degrees of freedom for elongated molecules.

For material related to this talk, click here.

A New Poisson-Boltzmann Equation for Two Types of Ion Species with Different Size

Prof. Chiun-Chang Lee

Recently, a wide variety of Poisson-Boltzmann (PB) type equations have been established to approach the phenomena of ion transport in various electrolyte solutions. Due to finite sized effect on the electric double layer at the surface, Andelman et. al. consider a modified Poisson-Boltzmann (MPB) equation for electrolyte solutions with two types of ions having the same size (cf. PRL, 1997). The MPB equation is a good model for describing the effect of ions' radii on the behavior of the electric double layer. However, in the case when different size ion species occupy electrolyte solutions, the MPB equation seems unavailable. The main purpose of this talk is to introduce a new PB equation with finite size effects, called the PB_ns equation. To briefly study this model, we are going to focus on the case of one cation and one anion species and formally derive a limiting form of the PB_ns equation which is more general than the MPB equation. In particular, when the size of all ions are the same, we show that solutions of the PB_ns equation and the MPB equation have the same asymptotic behavior in the limit of zero Debye length.

This is a joint work with Tai-Chia Lin and Chun Liu.

For material related to this talk, click here.

A Continuous Spectrum of Partial Differential Equations

Prof. Daniel Spector

The study of fractional and nonlocal partial differential equations has seen a renewed interest in recent years, as can be seen for example in the work of Caffarelli and Silvestre, as well as Sire, Valdinoci and others. In fact, the notion is much older, dating at least to work of Calderon and Zygmund. In this talk, I will review some of the history and relevant ideas, as well as discuss recent work on the subject done in collaboration with Tien-Tsan Shieh.

The existence of the weak solutions and the traveling waves to the hyperbolic and parabolic-hyperbolic Keller-Segel equations in chemotaxis.

Prof. Meng-Kai Hong

In this talk, we consider the general hyperbolic Keller-Segel equations in chemotaxis, which can be written as the hyperbolic systems of balance laws. We establish the global existence of the weak solutions to the Riemann and Cauchy problems by the generalized Lax method and the modified Glimm scheme. To the parabolic-hyperbolic K-S equations, we study the existence and the behavior of the traveling wave solutions by the technique of geometric singular perturbations. This is the joint work with J. S. Guo of Tamkang University and Y. S. Chen of National Central University

For material related to this talk, click here.

A Liouville theorem for the planar Navier-Stokes equations with the no-slip boundary condition and its application to a geometric regularity criterion

Dr. Pen-Yuan Hsu

In this talk, we establish a Liouville type result for a backward global solution to the Navier-Stokes equations in the half plane with the no- slip boundary condition. No assumptions on spatial decay for the vorticity nor the velocity field are imposed. We study the vorticity equations instead of the original Navier-Stokes equations. As an application, we extend the geometric regularity criterion for the Navier - Stokes equations in the three dimensional half space under the no-slip boundary condition. This is a joint work with Yoshikazu Giga (University of Tokyo) and Yasunori Maekawa (Tohoku University).

A numerical energetic variational approach for constructing spectral schemes for PNP model

Prof. Chun-Hao Teng

In this talk we will present a numerical procedure for constructing computa- tional schemes to simulate the dynamics of charge activities in ionic channel. Here we consider that the dynamics of charges is described by a PNP model satisfying an energy functional involving: (1) energy density functions of the ln ci with each ci representing a charge concentration, and (2) an form ci electrostatic potential represented by a convolution of a Green function and charge concentrations.

To illustrate the concepts in the present scheme construction procedure, we shall first based on a model wave problem, give a short discussion about the relationships between the energy estimate of the model problem and the numerical stability of a scheme for solving the wave equation. In the second part of the talk, we shall describe how to extend these concepts to construct a numerical scheme, based on pseudospectral penalty methods, for the PNP equations satisfying the aforementioned energy functional.

Localized waves in FitzHugh-Nagumo equations

Prof. Chao-Nien Chen

Patterns and waves are commonly observed in physical, chemi- cal and biological systems. Depending on the system parameters and initial conditions, dissipative structures may stay at rest or propagate with a dy- namically stabilized velocity. This talk is aimed at variational approach for studying localized waves in FitzHugh-Nagumo equations.

For material related to this talk, click here.

Qualitative studies of Lotka-Volterra competition system with advection

Prof. Qi Wang

In this talk, we consider a diffusive Lotka-Volterra competition system with advection under Neumann boundary conditions. Our model describes a relationship that one species escape from the region of high population density of inter-specific competitors in order to avoid competition. The global existence of bounded classical solutions are established for a parabolic-parabolic system over one-dimensional domains and for its parabolic-elliptic counterpart over multi-dimensional domains. We then study the existence and stability of non-constant positive steady states through bifurcation theories. As the diffusion and advection rate of the first competitor go to infinity, it is shown that this reaction-advection-diffusion system converges to a shadow system when . We construct positive solutions with an interior transition layer to the shadow system at any predetermined point over the given interval. Numerical simulations are presented to illustrate and support our theoretical results.

For material related to this talk, click here.

Multivariate Analysis of Angular Data

Prof. Carmay Lim

Our research interests are to

(i)unravel the principles governing biological processes and use them to identify novel drug targets and guide drug design,1,2 and

(ii) develop new methods for studying macromolecular interactions.

This talk will provide an overview of our work in these two areas. It will then describe multivariate analysis of angular data,3 including principal component analysis, k-means, hierarchical clustering, and linear regression designed for angular data.

References

1.Competition among metal ions for protein binding sites: Determinants of metal ion selectivity in proteins. Todor Dudev & Carmay Lim, Chem. Rev. (2014) 114: 538−556. http://dx.doi.org/10.1021/cr4004665

2.Factors Controlling the Role of Zn and Reactivity of Zn-bound Cysteines in Proteins: Application to Drug Target Discovery. Yu-Ming Lee, Yeh-fon Lin, and Carmay Lim, J. Chin. Chem. Soc. (2014) 61: 142-150. doi: 10.1002/jccs.201300392

3.GeoPCA – a new tool for multivariate analysis of dihedral angles based on principal component geodesics. Karen Sargsyan, Jon Wright & Carmay Lim, Nucleic Acids Res. (2011) 40: e25. doi:10.1093/nar/gkr1069

For material related to this talk, click here.

Computing structural and dynamic properties of biological systems at multiscale: protein function, membrane protein assembly, chromosome folding, stochastic networks of epigenetic states, cell and tissue patterning, and simulating wound healing(5)

Prof. Jie Liang

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It is our belief that this multi-scale approach will be useful for studying and engineering complex biological systems. (Please visit http://www.uic.edu/~jliang for further information).

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Dynamics, Randomness and Singularities in Genetics and Evolution

Prof. David Waxman

In these lectures I will present some dynamical models from genetics and evolutionary biology. The lectures will start from some very basic and elementary considerations. I will develop these into models of interest to biologists. We will first consider the properties and behaviour of systems with discrete states and randomness, reaching the Wright-Fisher model (which is a Markov chain that plays an important role in genetics). We will then consider continuous models, and use some results of these to study a continuous diffusion approximation of the Wright-Fisher model. This diffusion approximation is remarkably accurate and useful, and has some interesting and surprising properties. We will also consider some simple models of quantitative traits, which incorporate mutation and selection. If time allows, I will present a model of quantitative traits that shows a distinct transition, as a function of the dimensionality of the problem.

These lectures will concentrate on the description and dynamics of models where randomness plays an essential role. As we shall see, some of these models can lead to non-smooth (singular) distributions.

These lectures will be presented at a level of rigour (or non-rigour) that is commonly practised in theoretical physics and population genetics. In discussion sessions, we may wish to explore the different ways that mathematicians and theoreticians (i.e., researchers from other backgrounds), think about and analyse problems. In particular, we may discuss the degree to which different approaches leads to intuition which guides creativity and the understanding of new problems.

For material related to this talk, click here.

Dual gradient effects in chemotaxis: attraction vs. repulsion

Prof. Zhi-An Wang

Most of existing researches on chemotaxis models deal with attraction and repulsion separately. But in some biological processes, the repulsive process often follows the attraction to accomplish certain biological objectives. In such scenario, a chemotaxis model with combined attraction and repulsion will be more realistic. In this talk, we shall discuss the completing effects in an attraction-repulsion chemotaxis model describing aggregation of Microglia in Alzhemer's disease, and show various interesting behaviors resulting from the competition of attraction and repulsion, including global existence, blowup, critical mass phenomenon and pattern formations. Numerical simulation of pattern formations will be shown and open questions will be discussed.

For material related to this talk, click here.

Electrical and Structural Remodeling of Rabbit Ventricles during Therapeutic Hypothermia: Role of Conduction Velocity on Ventricular Arrhythmogenesis

Prof. Yu-Cheng Hsieh

Therapeutic hypothermia (TH, 30°C and 33°C) protects the brain from hypoxic injury in patients resuscitated from sudden cardiac death. Clinical guidelines accordingly recommend that unconscious adult patients with spontaneous circulation after out-of-hospital cardiac arrest should be cooled to 32–34°C for 12–24 h when the initial rhythm was ventricular fibrillation (VF). However, TH per se may potentiate the occurrence of lethal ventricular tachycardia (VT) and VF, while the mechanism remains unclear.

Cardiac electrical alternans, particularly spatially discordant alternans (SDA), is a key arrhythmogenic factor for the initiation of VT and VF. Whether SDA underlies the mechanism of TH-induced VF remains to be explored. During TH, conduction disturbance (slow conduction velocity and heterogeneous conduction) might cause unidirectional conduction block, leading to reentry ventricular tachyarrhythmia (VT/VF). One important determinant of cardiac conduction velocity is cell-to-cell coupling, which is mediated by gap junctions (GJs) constructed from connexin (Cx) proteins.

Whether GJ coupling in ventricles might have altered shortly after the implementation of TH, and consequently contributed to the conduction disturbance during TH remains to be investigated. We have previously found that severe hypothermia (30°C) creates an arrhythmogenic substrate that enhances the initiation (pacing-induced SDA) and maintenance (increased wavebreaks) of VF. Short-duration (30 min) TH also causes a prompt temperature-dependent Cx43 GJ remodeling, in which the PKC pathway is involved. In this talk, we will discuss our recent findings regarding the influence of ventricular conduction velocities on ventricular arrhythmogenesis during TH.

For material related to this talk, click here.

Transport of Charged Particles in Biological Environment: An Energetic Variational Approach(5)

Prof. Chun Liu

Almost all biological activities involve transport of ions through biological environments. The nature of these problems makes it necessary to couple effects from different scales, both spatial and temporal. Motivated by the seminal work of Rayleigh and Onsarger, together with the developments in the past 50 years on chemical engineering and soft matter physics, the general framework of energetic variational approaches is developed specifically to be consistent with the basic principles of statistical physics and non-equilibrium thermodynamics, and at the same time, incorporate the specific physical and biological ingredients/considerations in the models.

In this mini-course, I will go over some of the basic approaches in related to modern mathematical analysis and numerical techniques. In particular, due to the time constraint, I will focus on the derivation of some basic systems and the relation to the classical theories for idea materials.

Some of the topics that I wish to cover in the course:

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least action principle and maximum dissipation principle.

Navier-Stokes equations and elasticity.

2. Multiscale modeling and analysis:

basis of stochastic differential equations: Fokker-Planck equations, diffusion, Smoluchowski coagulation equations, variational formulations, kinetic theory.

micro-macro models for polymeric materials.

moment closure methods, Mori-Zwanzig formulation and other coarse grain methods.

3. Ionic fluids and ion channels:

generalized diffusion, nonlocal diffusion.

electroeheological (ER) fluids: Poisson-Boltzman fluids, steric effects of ion particles, equation of states.

ionic fluids in ion channels.

On a computational framework of studying needle/cell interaction in acupuncture manipulation - a preliminary study

Prof. Tony Wen-Hann Sheu

An on-going research in acupuncture will be presented in this talk. Three issues regarding the effect of needle manipulation on mast cell will be presented. The inter- action between the moving needle, with the mast cell will be presented first to yield a mechanical stress on cell membrane, cell degranulation and exocytosis, as a con- sequence of this mechanical gating, are then studied numerically. In this talk I will first summarize what have been done in Chinese medicine, namely, the macroscopic chi-blood interaction owing to acupuncture and moxibustion. For the three topics un- der current investigation, I will present their respective mathematical models, some preliminary simulation results, together with the mathematical analysis within the framework of Keller-Segel equation.

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Computing structural and dynamic properties of biological systems at multiscale: protein function, membrane protein assembly, chromosome folding, stochastic networks of epigenetic states, cell and tissue patterning, and simulating wound healing(3)

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Thinking about selection and drift in terms of trajectories(3)

Prof. David Waxman

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At the cellular level, we describe a dynamic finite-element cell (dFEMC) model and an algorithm for simulating time-evolving spatio-temporal pattern formation of cell populations. We discuss in details how universal topological distribution of sidedness of proliferating epithelia cells across species can be simulated, and how tissue elongation may be regulated by oriented division and oriented mechanical forces. To understand how proteins and networks inside individual cells lead to formation of global tissue patterns, we described in some details on how the process of wound healing can be studied using the dFEMC models, with explicit protein networks controlling growth/dvision, migration, apoptosis, and quiescence embedded inside each cell. We discuss simulation results of cell-cell interactions and cell-ECM interactions, including prediction of keartinocyte migration, formation of hyperproliferative zone, and effects of cytokines on speed of wound closure.

It is our belief that this multi-scale approach will be useful for studying and engineering complex biological systems. (Please visit http://www.uic.edu/~jliang for further information).

For material related to this talk, click here.

Thinking about selection and drift in terms of trajectories(1)

Prof. David Waxman

In physics we often talk about the trajectories of particles. We have well established laws (e.g., as written down by Newton) to govern their properties. We have different levels of description (classical, quantum, ...). In biology, in genetics and evolution in particular, we can also talk about trajectories. The trajectories are in a different space to the trajectories of physics, that I will introduce. There are also different levels of description, that are determined by the nature of the populations under consideration. In this talk I present some basic ideas of genetics and evolution in terms of trajectories. I will discuss the implications of conditioning on the dynamical description of a population, when observations tell us the initial and final points of a trajectory.

Transport of Charged Particles in Biological Environment: An Energetic Variational Approach(1)

Prof. Chun Liu

Almost all biological activities involve transport of ions through biological environments. The nature of these problems makes it necessary to couple effects from different scales, both spatial and temporal. Motivated by the seminal work of Rayleigh and Onsarger, together with the developments in the past 50 years on chemical engineering and soft matter physics, the general framework of energetic variational approaches is developed specifically to be consistent with the basic principles of statistical physics and non-equilibrium thermodynamics, and at the same time, incorporate the specific physical and biological ingredients/considerations in the models.

In this mini-course, I will go over some of the basic approaches in related to modern mathematical analysis and numerical techniques. In particular, due to the time constraint, I will focus on the derivation of some basic systems and the relation to the classical theories for idea materials.

Some of the topics that I wish to cover in the course:

1. General energetic variational framework for complex fluids:

least action principle and maximum dissipation principle.

Navier-Stokes equations and elasticity.

2. Multiscale modeling and analysis:

basis of stochastic differential equations: Fokker-Planck equations, diffusion, Smoluchowski coagulation equations, variational formulations, kinetic theory.

micro-macro models for polymeric materials.

moment closure methods, Mori-Zwanzig formulation and other coarse grain methods.

3. Ionic fluids and ion channels:

generalized diffusion, nonlocal diffusion.

electroeheological (ER) fluids: Poisson-Boltzman fluids, steric effects of ion particles, equation of states.

ionic fluids in ion channels.

Computing structural and dynamic properties of biological systems at multiscale: protein function, membrane protein assembly, chromosome folding, stochastic networks of epigenetic states, cell and tissue patterning, and simulating wound healing(2)

Prof. Jie Liang

Understanding and manipulating the machineries of cells and tissues requires a multi-scale approach that examines details of individual proteins, interactions of multiple proteins, and genetic circuit networks to elucidate complex behavior of cellular and tissue states and the formation of their spatio-temporal patterns in health and disease.

At the molecular level, we discuss how to compute protein geometric structures, including the characterization of voids and pockets, and the origin of their existence. We further illustrate how to predict protein functions by comparing local surfaces at large scale through reconstruction of the evolutionary history of binding surfaces using a continuous-time Markov model and a Bayesian Monte Carlo estimator. We also describe studies of structures, assemblies, and thermodynamic properties of beta barrel membrane proteins. Based on a model of physical interactions, a discrete state space, and an empirical potential function derived from detailed combinatorial analysis of protein structures, as well as a model to account for inter-strand loop entropy, we discuss prediction of structures of TM-segments and loops, oligomerization states, protein-protein interaction interfaces, transfer free energy scales, folding stability, and protein topological orientation, as well as general stabilization strategies that is applicable for design of stable bionanopore.

At the network level, we describe a method for optimal enumeration of the state space of a stochastic network and the mb-dCME method we developed for direct solution of the discrete chemical master equation (dCME) that can account for full stochastic control of rare and small copy-number events, which are often important for determining critical biological phenomena such as cellular fate. We will also discuss the computation of the exact time-evolving probabilistic landscape without Gillespie simulation or Fokker-Planck/Langevin approximation. We report discoveries of complex multistable landscapes arising from simple network motifs, without requring feedback loops or cooperativities that were often thought to be obligatory. We show how to relate the computed landscape probability to phenomenological characterization of the decision networks in phage-lambda such as bi-stability, epigenetic states, and the robustness of wild type versus mutants of phage lambda.

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ionic fluids in ion channels.

Mesoscopic Stochastic Nonequilibrium Thermodynamics, entropy production, and kinetic cycles.

Prof. Hong Qian