

**2015 International Workshop on
Computational Science and Engineering**

Date: May 23rd (Sat), 2015

Place: Room ES033 at ES building, Nagoya University, Japan
ES building (C2 on the map)

Program

May 23rd (Sat)

8:55 - 9:00

Opening

Chair (9:00-10:30): Tomohiro Sogabe

9:00 - 9:30

Michael Ng

Non-negative tensor equations: applications and algorithms

9:30 - 10:00

Katsunori Yoshimatsu

Influence of vortex dynamics and structure on turbulence statistics at large scales with or without combustion

10:00 - 10:30

Can Yang

Shared genetic architecture between psychiatric disorders and autoimmune disorders revealed by statistical analysis of Big Data in Biomedicine

10:30 - 10:45

Break

Chair (10:45-12:15): Takashi Ishihara

10:45- 11:15

Naoya Okamoto

Applications of wavelet analysis to turbulence

11:15 - 11:45

Henry Y. T. Ngan

A Comparative Study of Outlier Detection for Large-scale Traffic Data by one-class SVM and Kernel Density Estimation

11:45 - 12:15

Tomoki Terada

Coupling between phosphorylation rhythm and ATP hydrolysis rate in KaiC protein studied by stochastic simulation

12:15 - 14:00

Lunch

Chair (14:00- 15:30): Sung Nok Chiu

14:00 - 14:30

Noriyuki Yoshii

All-atom molecular dynamics calculation study of entire poliovirus empty capsids in solution

14:30 - 15:00

Tieyong Zeng

Convex and non-convex variational models for image restoration and segmentation

15:00 - 15:30

Shingo Kobayashi

Topological classification of vortices and monopoles in condensed mattersystems

15:30 - 15:45

Break

Chair (15:45- 17:15): Chin Ko Yau

15:45 - 16:15

Chi Man Leung

A numerical algorithm on pricing of contingent convertible with Parisian feature

16:15 - 16:45

Yuto Miyatake

Geometric numerical integration methods for evolution equations and their recent development

16:45 - 17:15

Felix Kwok

Schwarz Methods for the Time-Parallel Solution of Parabolic Control Problem

17:15 - 17:20

Closing

18:30 -

Banquet

Non-negative tensor equations: applications and algorithms

Michael Ng (Hong Kong Baptist University)

In this talk, I introduce non-negative tensor equations in data mining and community discovery. I will present the relevant algorithms and experimental results of these applications.

Influence of vortex dynamics and structure on turbulence statistics at large scales with or without combustion

Katsunori Yoshimatsu (Nagoya University)

Turbulence is ubiquitous in our daily life. Most vorticity in fully developed turbulence at high Reynolds number resides at small scales in the so-called energy dissipation range, while most turbulent kinetic energy is at the scales in the so-called energy containing range that is at scales much larger than those in the dissipation range. We first examine the influence of small-scale vortex dynamics and structure on turbulence statistics at large scales without chemical reaction, using so-called computational surgery. It is found that the statistics at large scale are insensitive to the details of the vortex dynamics and structure, at least in the case studied here. The insensitivity is quite encouraging to turbulent models, e.g., large eddy simulation which computes only the large-scale evolution, while modeling the influence of small-scale motion onto the large-scale motion. For turbulence with combustion, its small-scale vortex dynamics are very active, because the chemical reaction occurs at smaller scales. This suggests the difficulty of modeling turbulent combustion. Its dynamics and structure play important roles in enhancement/suppression of the reaction.

Shared genetic architecture between psychiatric disorders and autoimmune disorders revealed by statistical analysis of Big Data in Biomedicine

Can Yang (Hong Kong Baptist University)

Although some existing epidemiological observations and molecular experiments suggested that brain disorders in the realm of psychiatry may be influenced by immune dysregulation, the degree of genetic overlap between psychiatric disorders and immune disorders has not been well established.

The rise of Big Data in genomics provides us unprecedented opportunities to address the above scientific hypothesis. Nowadays, multilayered genomic data carry much richer information than ever. On one hand, several recent international projects, such as the Encyclopedia of DNA Elements (ENCODE) project, have generated vast amounts of genomic data measured at the cellular layer, i.e., cellular traits, including chromatin states and gene expression levels in different tissues. On the other hand, genome-wide association studies (GWAS) have genotyped millions of genetic variants (i.e., SNPs) and surveyed hundreds of organismal traits, such as height, weight, blood pressure and disease status. How to integrate multilayered data (SNPs, cellular traits and organismal traits) becomes an essential step to deepen our understanding of biological basis of complex diseases.

In this talk, we introduce a novel statistical approach, GPA (Genetic analysis incorporating Pleiotropy and Annotation), to increase statistical power to identify risk variants through joint analysis of multiple GWAS data sets and annotation information. Statistical inference of the model parameters and SNP prioritization are achieved through an expectation-maximization (EM) algorithm that can handle genome-wide data efficiently. The R implementation of GPA is currently available at <https://sites.google.com/site/eeyangc/software/gpa>.

With the GPA approach, we performed integrative analysis of genome-wide association studies of 18 complex human traits/diseases (five psychiatric disorders, seven autoimmune disorders, and others) and multiple genome-wide annotation resources (Central nervous system genes, immune-related expression-quantitative trait loci (eQTL) and DNase I hypersensitive sites from 98 cell-lines). We detected pleiotropy in 24 of the 35 psychiatric-autoimmune disorder pairs. The strongest pleiotropy was observed for schizophrenia-rheumatoid arthritis with MHC region included in the analysis ($p=3.9e-285$), and schizophrenia-Crohn's Disease with MHC region excluded ($p=1.1e-36$). Strong enrichment (>1.4 fold) of immune-related eQTL was observed in four psychiatric disorders. Genomic regions responsible for pleiotropy between psychiatric disorders and autoimmune disorders were detected. The MHC region on chromosome 6 appears to be the most important with other regions, such as cytoband 1p13.2, also playing significant roles in pleiotropy. We also found that most alleles shared between schizophrenia and Crohn's disease have the same effect direction, with similar trend found for other disorder pairs, such as bipolar-Crohn's disease.

Applications of wavelet analysis to turbulence

Naoya Okamoto (Nagoya University)

Turbulence, ubiquitous in our daily life, is still one of the most challenging problems in science. Turbulence exhibits an intrinsic multiscale behavior due to a large number of degrees of freedom interacting nonlinearly. Observations show its self-organization into vortices superimposed to a background flow. This motivates us to split turbulent flows into two contributions, i.e., coherent vortices and a random background flow. Both contributions are multiscale and exhibit no scale separation. To reduce the computational load for simulating turbulent flow, the coherent vorticity simulation (CVS) method, which retains only the flow induced by the coherent vortices, has been proposed. In this talk, we briefly review a wavelet filtering technique used in CVS and assess the potential of CVS for three-dimensional homogeneous isotropic turbulence.

A Comparative Study of Outlier Detection for Large-scale Traffic Data by One-class SVM and Kernel Density Estimation

Henry Y.T. Ngan (Hong Kong Baptist University)

This talk aims at presenting a comparative study of outlier detection (OD) for large-scale traffic data. The traffic data nowadays are massive in scale and collected in every second throughout any modern city. In this research, the traffic flow dynamic is collected from one of the busiest 4-armed junction in Hong Kong in a 31-day sampling period (with 764,027 vehicles in total). The traffic flow dynamic is expressed in a high dimension spatial-temporal (ST) signal format (i.e. 80 cycles) which has a high degree of similarities among the same signal and across different signals in one direction. A total of 19 traffic directions are identified in this junction and lots of ST signals are collected in the 31-day period (i.e. 874 signals). In order to reduce its dimension, the ST signals are firstly undergone a principal component analysis (PCA) to represent as (x,y)-coordinates. Then, these PCA (x,y)-coordinates are assumed to be conformed as Gaussian distributed. With this assumption, the data points are further to be evaluated by (a) a correlation study with three variant coefficients, (b) one-class support vector machine (SVM) and (c) kernel density estimation (KDE). The correlation study could not give any explicit OD result while the one-class SVM and KDE provide average 59.61% and 95.20% DSRs, respectively.

Coupling between phosphorylation rhythm and ATP hydrolysis rate in KaiC protein studied by stochastic simulation

Tomoki P. Terada (Nagoya University)

KaiC protein shows circadian oscillation of phosphorylation level in vitro in the presence of KaiA, KaiB and ATP. As this Kai system is the simplest circadian rhythm consisting of only proteins, its mechanism has been intensively studied where the circadian rhythm has been ascribed to collective dynamics of protein molecules in different states.

However, it has been shown later that the frequency of this circadian oscillation strongly correlates with ATP hydrolysis rate of KaiC in the absence of KaiA or KaiB, the latter of which does not show any circadian rhythm.

Here we propose a single molecule model of KaiC with a large number of states. Stochastic simulation of this single molecule model has revealed that coupling between structural states and chemical states of KaiC can lead to the experimentally observed correlation between phosphorylation rhythm and ATP hydrolysis rate.

All-atom molecular dynamics calculation study of entire poliovirus empty capsids in solution

Noriyuki Yoshii (Nagoya University)

Large-scale (6.5 million atoms) and long-time (200 ns) all-atom molecular dynamics (MD) calculations for poliovirus empty capsid were conducted using the K-computer and highly parallelized general purpose MD simulation software MODYLAS. We clarified a molecular origin of stability of virus capsid. The solutions inside and outside of the capsid converged well to the equilibrium states. The equilibration of MD calculation was also confirmed by the fact that the water molecules pass through the capsid from one side to the other at the same rate for both directions. In equilibrium, the solution density inside capsid was lower than that in outside. The local pressure inside the empty capsid was -2.8 ± 0.3 and -3.4 ± 0.5 MPa from the pressure-density relationship and virial theorem, respectively. The both results show that the local pressure inside the capsid is negative. From the detailed analysis, the negative pressure was found to come from the coulombic interaction of negative excess charges of the capsid. This leads to the instability of the empty capsid. The negative pressure must be compensated by positive contributions by the RNA and its counterions. Stabilization of the capsid by the RNA may thus be understood from the viewpoint of the pressure as a measure of stability and instability.

Convex and non-convex variational models for image restoration and segmentation

Tieyong Zeng (Hong Kong Baptist University)

In this talk, I introduce convex and non-convex models in image restoration and segmentation. I will present the relevant theories and algorithms with applications.

Topological classification of vortices and monopoles in condensed matter systems

Shingo Kobayashi (Nagoya University)

Topology is now considered to be an important guiding principle in condensed matter physics. Topological objects appear in various systems such as ultracold atomic systems and unconventional superconductors, and ones remain invariant under a small symmetry-preserving perturbation due to a topological invariant. The purpose of this presentation is to show how to classify these topological objects using the homotopy theory, which is the most suitable mathematical tool to define the topological invariant. I also discuss applications of the homotopy theory to topological excitations in real space and nodal structures of an unconventional superconductor in momentum space.

A numerical algorithm on pricing of contingent convertible with Parisian feature

Chi Man Leung (Hong Kong Baptist University)

Contingent convertible bonds (CCBs) is one of popular financial instruments used by the firm to raise capital for running its businesses. Different from standard convertible bonds, the contingent convertible bonds will convert into equity automatically when the firm is under financial distress and the firm is prevented from default. In this talk, we will develop a pricing model and examine the pricing procedure of the CCBs which the mandatory conversion occurs when the Tier-1 capital ratio either hit a barrier level from above or below a monitoring level (above barrier level) continuously for a period of time. Under the existence of Parisian feature embedded in the CCB, it is not efficient to obtain numerical approximation to the pricing formula using classical methods such as lattice tree approximation, Monte Carlo simulation and finite difference method because of curse of dimensionality. In this talk, we will also develop an efficient algorithm, via Fortet algorithm, to obtain the numerical approximation to the pricing formula of CCBs. Some special modifications (multi-stage approach and dimension reduction technique) are introduced to enhance the efficiency of the algorithm. We will also explore the pricing behavior of the CCBs with respect to various parameters.

Geometric numerical integration methods for evolution equations and their recent development

Yuto Miyatake (Nagoya University)

In this talk, we consider numerical methods for evolution equations. Geometric numerical integration methods are rather specific-purpose methods in the sense that they exactly preserve or inherit geometric properties, such as energy-preservation and symplecticity, of differential equations. The main advantage of geometric numerical integration methods is that in many cases we can expect qualitatively better numerical solutions, especially over a long period of time, than with general-purpose methods. In this talk, we briefly review basic concepts of geometric numerical integration methods, and show recent development especially for partial differential equations.

Schwarz Methods for the Time-Parallel Solution of Parabolic Control Problems

Felix Kwok (Hong Kong Baptist University)

Discretized parabolic control problems lead to very large systems of equations, because trajectories must be approximated forward and backward in time. It is therefore of interest to devise parallel solvers for such systems, and a natural idea is to apply Schwarz preconditioners to the large space-time discretized problem. The performance of Schwarz preconditioners for elliptic problems is well understood, but how do such preconditioners perform on discretized parabolic control problems? We present a convergence analysis for a class of Schwarz methods applied to a model parabolic optimal control problem. We show that just applying a classical Schwarz method in time already implies better transmission conditions than the ones usually used in the elliptic case, and we propose an even better variant based on optimized Schwarz theory.

INFORMATION

Lunch

Chez Jiroud

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Chez Jiroud (ES Building 1F)

Banquet

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