NTU Mathematics Colloquium

演講者：Prof. Jie Liang (University of Illinois, Chicago)

講　題：Topological Analysis of Structures-Dynamics of Biomolecules and Probabablistic Landscape of Cellular Fate: Computing Knots, Betti Numbers, and Persistent Homology

時　間：2019年12月9日 (星期一) 14:10-15:00

地　點：臺灣大學天數館 202 室

摘　要：Biomolecules and their reaction networks are the basis of cellular functions. We discuss how better understanding of structures and dynamics of biomolecules, as well as the behavior of their interaction networks can be gained from topological analysis. For three-dimensional structures of biomolecules, we describe how stems of RNA molecules as well as disulfide bonds of proteins can be understood from a new class of knot polynomials. We also discuss how the opening and closing probabilities of ion channels can be quantified from rapid computation of betti numbers of computationally simulated ensemble of structures of ion channels with complex loop interactions. For dynamics of biomolecules, we show how identification of birth and death of 0-th homology group on a 5D free energy surface leads to the discovery of transition states of a chemical isomerization reaction. For networks of interacting biomolecules, we show how exact probability surface of stochastic chemical kinetics can be computed via the ACME (acme.org) method by solving the chemical master equation. We then discuss how a full topological treatise of the probability landscapes of stochastic networks is now feasible. We describe recent results in analysis of probabilistic landscape of networks of feed-forward loops and repressilator systems, including computation of persistent homology, detection of k-cycles and topological changes. We also highlight key challenges in computing persistent homology of high-dimension scalar surface.

茶　會：15:00-15:30

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