

RYERSON UNIVERSITY
DEPARTMENT OF MATHEMATICS
BIOMATHEMATICS & FLUIDS SEMINAR

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Date: Thursday, February 11, 2016

Time: 2:15pm

Location: ENG 288

**Stochastic Micro- and Mesoscale Simulations
of Biochemical Reaction-Diffusion Systems**

Abstract:

In this talk, I will introduce two stochastic computational approaches for simulating biological signaling pathways at a micro-/mesoscale level: The first approach is discrete in space and continuous in time and builds upon the widely used Inhomogeneous Stochastic Simulation Algorithm (ISSA) by simulating a corresponding Reaction-Diffusion Master Equation. ISSA is known to be exact but computationally expensive. The newly developed (hybrid) approach decreases the computational runtime significantly while maintaining high accuracy. I will present some benchmark studies for biochemical reaction-diffusion models and discuss ideas for further applications to general transport problems at cell level.

The second approach is a particle-based method that monitors single constituents that are continuous in space. In the literature it is mostly referred to as Multi-Particle Collision (MPC) Dynamics or Stochastic Rotation Dynamics (SRD). The collisions model diffusion transport and obey physical laws of conservation. MPC is known to be computationally more efficient than many other particle-based collision models. I will demonstrate recent applications to intracellular pathways for chemotaxis and address some open challenges. This work is a result of joint collaboration with Silvana Ilie and Katrin Rohlf at Ryerson University.

ALL FACULTY, STAFF, STUDENTS AND GUESTS ARE WELCOME TO ATTEND