MATH 793I – Fall 2017

Spatial Stochastic Simulations of Bio-Molecular Processes

Time & Location **TuTh 11:30 – 12:45; 313 Armstrong Hall (NOTE NEW TIME)**

Instructor: **Adam Halasz**, PhD, Associate Professor, WVU Mathematics

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Text: Notes and free (open access) materials, such as reviews, tutorials, or published articles.

Objective: This is a beginning graduate level introduction to particle based **modeling and simulation of reaction-diffusion systems in two (or more) spatial dimensions**, with focus on processes and methods relevant to molecular systems biology. *A background in biology is useful but not required*. The core of the course deals with probabilistic (stochastic) models describing a class of molecular processes, with emphasis on *Monte-Carlo simulations* of biochemical reactions on the surface of living cells. At the end of the course, students will understand and be able to construct basic stochastic simulation algorithms of chemical reactions and reaction-diffusion processes. Students familiar with Matlab® (or a programming language) will be able to implement such simulations.

Intended audience: The course continues the two semester *Mathematical Systems Biology* sequence offered in the past years. However, this is designed to be a **stand-alone introduction to spatial stochastic models** and only requires familiarity with dynamical systems and basic multivariate calculus. Depending on student interest, we may follow a theoretical or applicative path. The theoretical side will emphasize the connection between the particle (agent based) and continuum picture of diffusion-reaction systems and focus on the consistency of algorithms. Students with basic working knowledge of a programming language may opt for an applicative path, emphasizing implementation and writing Monte Carlo simulation code.

The course is intended for graduate students in **Mathematics** (Differential Equations major and applied), as well as students in **Engineering, Physical** or **Life Sciences** interested in quantitative biology or Monte-Carlo simulations. For those interested in applications, projects will involve Matlab® or another programming language.

Content: A tentative list of topics to be covered*:

1. *Introduction / review of Cell Biology for Non-Biologists*
2. *Chemical reactions – a quick summary*
   - *Traditional (ODE) picture*
   - *Stochastic picture*
3. *Non-spatial simulation of chemical reactions as random processes*
   - *Gillespie SSA and its variants (such as τ-leaping)*
   - *Rule based approach for complex reaction networks*
4. *Brownian motion and diffusion*
   - *Connection between the fluid and particle based picture*
   - *Brownian Motion simulations*
   - *Lattice based simulations (optional – time permitting)*
5. *Simulating reaction-diffusion systems*

Grading*: Homework (20%), participation (10%), two midterm projects (40%), final project (30%).

Inclusivity: **The West Virginia University community is committed to creating and fostering a positive learning and working environment based on open communication, mutual respect, and inclusion. If you are a person with a disability and anticipate needing any type of accommodation in order to participate in this class, please advise me and make appropriate arrangements with the Office of Accessibility Services (293-6700). For more information on West Virginia University's Diversity, Equity, and Inclusion initiatives, please see http://diversity.wvu.edu.**

*subject to small changes and adjustments; this version compiled on August 8, 2017

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