Spatiotemporal Modeling and Simulation

01 :: Introduction
Topic

Administration and Introduction

Program

Organization of the lecture
Organization of the exercises
Talk: why simulations / concrete examples
Self-test questions
Learning goals

Be familiar with the organization of the lecture and the exercises

Have seen several examples of spatio-temporal modeling in biology

Know when and why to use modeling

Know about the limitations and issues
But first of all: who are these guys??

--- lecture ---
Ivo Sbalzarini <ivos@mpi-cbg.de>

--- exercises ---
Karl Hoffmann <karlhoff@mpi-cbg.de>

MOSAIC Group
mosaic.mpi-cbg.de
Lecture syllabus

1: Admin & Intro
2: Dimensionality analysis, slow and fast dynamics
3: Reservoirs and Flows, Causality diagrams
4: Recap on vector analysis
5: Conservation Laws, Control volume methods, how to derive PDEs
6: Particle methods, Function and Operator approximation
   hybrid and pure, interpolation
7: Diffusion, RW, PSE
8: Reaction-Diffusion, coupling with ODEs, Gillespie Algorithm
9: Advection-Diffusion, moving particles, remeshing
10: Flow, Vortex Methods
   (Advection with implicitly determined velocity field)
11: PDEs: classification, characteristics

No lecture on May 7, May 21 (Pentecost), July 9 + 16
Exam

120 minutes written

Semester-end exam

8 pages of hand-written summary or computer-written in font >8 pt.

Can replace Rigorosum at Fac. Bio.
Lecture web page

http://mosaic.mpi-cbg.de/?q=education/courses/STMS

You can find there:

Program
Slides, Scripts, Papers, Self-check questions, Code
Exercises

Time and Location: Agree with Tutor.

First time next week.

Rigorosum conditions:
- Successfully passing the exam
Exercises (cont.)

Organization:

- Work on the exercise sheets

- Weekly exercise sheets (paper and pencil / computer programs)

- Project building and simulating a biological model using the studied concepts
Exercise topics:

- Dimensionality analysis from a biological fluid mechanical system
- Slow/Fast dynamics from enzyme kinetics
- Identification of flows and reservoirs in the student project, Causality diagrams
- Some exercises on linear algebra, analysis of steady states
- Conservation in 1D and 3D to get a PDE, derivation of the equations for the student project
- Implementation of efficient data structures for particle simulations
- Different implementation of diffusion, e.g. random walks in different dimensions, Particle strength exchange (PSE) method
- Modeling reaction-diffusion-advection in the QS system
- Identification of PDE classes in dependence of the system coefficients
Project related exercises: Quorum sensing in V. fischeri
Quorum sensing in V. fischeri

- V. fischeri is a marine bacterium. They are luminescent when the population reaches a critical density (= quorum)

- We will study a model that describes this phenomenon based on:
Quorum sensing in V. fischeri

The model inside a bacterium:

Fig. 1 Scheme of the regulatory pathway
Quorum sensing in V. fischeri

Cell-cell communication:
Quorum sensing in V. fischeri

Real image of a luminescent population: