0. Sunday August 11, 2019 Python

10:00 – 10:30AM **Welcome** (James A Glazier)

10:30 – 11:00AM **Install Tellurium or Other Python IDE (Endre Somogyi)**

10:00 – 12:30PM **Introduction to Python (Endre Somogyi)**

12:30 – 1:00PM Lunch [provided]

1:30 – 2:30PM **Introduction to Python (Endre Somogyi)**CC3D installation check

2:30 – 3:15PM **Overview of cell-based tissue modeling** (James Glazier) attendees will gain information about how CC3D and multi-scale modeling can be applied to a variety of biological systems.

3:15 – 5:00PM **Group Model Scoping**

As a group we will discuss each attendees proposed model for ~30 minutes. Attendees should be prepared to describe their research questions, available data. Through this discussion we will define each attendees specific modeling goals for this workshop.

5:00 –5:15PM CompuCell3D Version 4 Installation Check

[Dinner on your own]

1. Monday August 12, 2019 Cell Behaviors

9:00 – 10:00AM **Group Model Scoping**

As a group we will discuss each attendees proposed model for ~30 minutes. Attendees should be prepared to describe their research questions, available data. Through this discussion we will define each attendees specific modeling goals for this workshop.

10:00 – 10:30AM **Discuss Possible Collaborative Projects**

Doing this model scoping collaboratively will support peer-to-peer collaboration among individuals with similar research questions.

10:30 – 11:15AM **Discussion about prior background (specifically R/K)**?

10:30 – 10:45AM **Break**

10:45 – 11:15AM **CC3D background, Twedit++, CC3D Player. Understanding the structure of CC3D simulations; Getting comfortable with CC3D Python scripting** (Maciej)

11:15 – 12:30PM **Avascular Tumor Spheroid Demo** (Juliano Ferrari) [(Diffusion, death, growth, uptake]

Key idea of phenomenological behaviors and interactions and their parameterization.

- Introduction to Chemical Diffusion Solvers in CC3D
- Chemical Field Sources
  - boundary, stromal tissue, blood vessels
- Where and how does chemical field disappear?
  - Decay (everywhere)
  - Consumption
    - Fractional/constant
  - How much chemical field is available per cell?
- How fast does the chemical field diffuse?
  - Relaxation time and equilibration time
- How far does the chemical field diffuse?

- As a function of size of domain what's minimum and maximum concentration?

12:30 – 1:00PM **Lunch** [provided]

1:00 – 2:30 **Explaining cells behaviours as a set of rules**

- Cell Growth
- Cell Death
- Cell Differentiation
- Cell Division

2:30 - 2:45 **Break**

2:45 – 4:15 **Avascular Tumor Model (putting things together)**

- Graphs of outputs
  - Number of proliferating, quiescent, necrotic cells
  - Growth rate
  - Total tumor size
- What controls growth
- Matching cell division/death/differentiation to concentration fields

4:15 – 4:30 **Break**

4:30 – 6.00 **Individual Model Development**

6:15 **Group Dinner** [at participant expense, Little Tibet Restaurant]

2. Tuesday August 13, 2019 Cellular Signaling

9:00 – 10:30 **Introduction to Cellular Signaling (Tellurium, SBML, LibRoadRunner)**

- Introduction: Integrating CompuCell3D and Subcellular Models (Julio)
- Introduction to Reaction Kinetics (Andy)
  - What are biological chemical reaction networks? What are their types and what do they do?
  - Representing biological networks mathematically and computationally (as ODEs/Gillespie)
- Solving Reaction Kinetics Models (Andy)
  - Introduction to Tellurium, SBML and LibRoadRunner
- Exporting Tellurium models as SBML. Importing SBML models into Tellurium. (Andy)
  - Coding a Cell Cycle model and exporting to SBML format

10:30 – 11:00 **Break**

11:00 – 12:15 **Cellular Signaling part 2 (creating multi-scale models in CC3D)**

- Biochemistry and Math behind Delta-Notch patterning Models (Julio)
  - Creating a multi-scale model of Delta-Notch patterning in CompuCell3D
  - Exercise: exploring variations in Delta-Notch model implementation
- Coupling cell-cycle models with CompuCell3D (Julio)
  - Goldbeter's Cell Cycle model
  - Tyson and Novak's Cell Cycle model
- Exercise: Combining Tyson's Cell Cycle with Collier's Delta-Notch models

12:15 – 1:00 **Lunch** [provided]

1:00 – 2:30 **Pharmacokinetic (PK) and Physiologically based pharmacokinetic modelling (PBPK)** (Jim Sluka)

2:30 – 2:45 **Break**

2:45 – 4:15 **Vascularization Demo** (Gilberto)

- Branching Morphogenesis
- Chemotaxis
- Custom field visualizations

4:15 – 4:30 **Break**

4:30 – 6:00 **Individual Model Development + Attendee Modeling Updates** (Stand-up style)

3. Wednesday August 14, 2019 Special Topics & Continued Model Development

9:00 – 10:30 **Effective use of CC3D** (Jim Sluka)

- Separating parameters from the code
- Running multiple simulations
- Logging results
- Running and interpreting parameter sensitivity scans

10:30 – 11:00 **Break**

10:15 – 12:15 **Individual Model Development**

12:15 – 1:00 **Lunch** [provided]

1:00 – 2:00 **Intestinal Crypt Model** (Furkan)

2:00 – 2:15 **Break**

2:15 – 4.30 **Individual Model Development**

4:30 – 6.00 **Attendee Modeling Updates** (Stand-up style)

[Dinner on your own]

4. Thursday August 15, 2019 Intermediate CC3D

9:00 – 10:30 **Wound healing** (Juliano and Julio)

- Growth and Mitosis, recap
- Contact inhibition of growth
- Wound healing based on adhesion
- Collective motion

10:30 – 11:00 **Break**

11:00 – 12:15 **Implementing Cell Crawling in CC3D** (Gilberto)

12:15 – 1:00 **Lunch** [provided]

1:00 – 3:00 **Individual Model Development**

3:00 – 3.15 **Break**

3:15 – 4.30 **Individual Model Development**

4:30 – 6.00 **Attendee Modeling Updates** (Stand-up style)

[Dinner on your own]

5. Friday August 16, 2019 CC3D in practice

9:00 – 10:00 **Parameterization, optimization, parameter scans, uncertainty quantification in CC3D** (Jim Sluka)

10:30 – 10:45 **Break**

10:45 – 12:15 **Particle Swarm Parameter Fitting Demo** (Jim Sluka)

12:15 – 1:00 **Lunch** [provided]

1:00 – 3:00 **Individual Model Development**

3:00 – 3.15 Break

3:15 – 4.30 **Individual Model Development**

4:30 – 6.00 **Attendee Modeling Updates** (Stand-up style)

[Dinner on your own]

6:15 **Optional Group Dinner and Drinks** [at participant expense, location to be announced]

6. Saturday Aug 17, 2019 Private tutorials and collaborations

Held in Simon Hall 047—Contact Somogyi, Belmonte and Glazier for access information

10:00 – 4:00 **Start, flexible schedule for the rest of the day**

[Meals on your own]

Course Instructors

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