Sub-cellular and Multicellular Modeling Workshop
at Indiana University, IN, USA

Instructors: Herbert M. Sauro (Univ. Washington), Maciej Swat, James Glazier, Andy Somogyi, Jim Sluka (Indiana Univ.)

The following materials will be provided to Participants during the Course:

1. *Discounted copy of Text Book on Enzyme and Gene Regulatory Kinetics (Paper and ebook)*
2. *CompuCell3D Introduction (all other manuals including CC3D reference, Python scripting etc… will be available in the electronic form)*
3. *PowerPoint/PDF copies of lecture slides*
4. *Folder with simulation notes and other materials*
5. *Model Files from the course web site*
6. *Selected readings and background material*

Aug 9th, 2015 (Sunday)

Introduction to Python Programming (optional):
Instructors: Andy Somogyi, Maciej Swat

Day 0: Course: 10AM – 5.00PM:

10.00 – 11.00: *Basic Python Programming (if, for, list, dictionaries etc…)*

11.00 – 12.00: *Basic Python Programming - Tutorials*

12.00 – 1.00: *Lunch Break*

1.00 – 2.00: *Slightly More Advanced Python Programming (classes and objects)*

2.00 – 3.00: *Slightly More Advanced Python Programming Tutorials*

3.00 – 3.15: *Break*

3.15 – 4.15: *Python Standard Library (file I/O, file management - os, path modules, sys module, search paths etc…)*

4.15 – 5.00: *Python Standard Library Tutorials*

Aug 10th, 2014 (Monday)

Day 1: Course: 9AM – 6.00PM:
Instructors: Herbert Sauro, Andy Somogyi

9.00 – 9.30: *Welcome note (James Glazier, Indiana Univ.)*

9.30 – 10.00: *Lecture:*
> *a) Introduction to Modeling with JDesigner and Jarnac*
> *b) Definitions of: Stoichiometry, Rate Laws,*
> *Boundary Species, Steady States and Transients*

10.05-10.30: *Hands on exercises*
> *a) Getting Help: Documentation and tutorials*
> *b) Simple Closed Systems*
> *c) Rate Law Selection*

10.30 – 11.00: *Break*

11:00 – 12:30: *Hands on exercises*
> *a) Simple Open Systems*
> *b) Applying Perturbations*
> *c) Plotting Simulations*
> *d) SBW Simulation Tool*

12.30 – 1.30: *Lunch*

1.30 – 2.30: *Lecture:*
> *SBML, Sensitivity Analysis, Parameter Scans*

3.30 – 4.00: *Break*

4:00 – 5:40: *Hands on exercises*
> a) Exchanging models, SBML, Matlab
> b) Using other models, obtaining model components
> c) Sensitivity Analysis, Interactive Modeling and Parameter Scans

5.40 – 6.00: *Road map for 2012-2014 and developer information*

Aug 11th, 2014 (Tuesday)
Day 2: Course: 9AM – 5.30PM:
Instructors: Herbert Sauro, Andy Somogyi
9.00 – 10.30: *Generalized enzyme kinetic rate laws*
9.35 – 10.30: *Mini Project: Build a Signaling Pathway*
10.30 – 11.00: *Break*
11:00 – 12:30: *Mini Project: Build a Signaling Pathway*
12.30 – 1.30: *Lunch*
1.30 – 5.30: *Mini Project: Build a Signaling Pathway, and Q&A session on Reaction Kinetics Modeling*

August 12th, 2014 (Wednesday)
Day 3: Course: 9AM – 5.30PM:
Instructors: Maciej Swat, James Glazier, Jim Sluka, Xiao Fu, Gui Oliveira, Andy Somogyi
9.00 – 10.30: *Overview of multi-cell modeling (James Glazier, Indiana Univ.)*
10.30 – 11.00: *Break*
11.00 – 12.30: *Introduction to CompuCell3D (Maciej Swat, Indiana Univ.)*
12.30 – 1.30: *Lunch*
1:30 – 3.00: *CompuCell3D 101 tutorials*
3:00 – 3.30: *Break*
3:30 – 5.30: *CompuCell3D (Introduction to Python-based Simulations-Mastering Twedit++, Python Mini-Tutorial, CC3D-Hands-on Exercises)*

August 13th, 2014 (Thursday)
Day 4: Course: 9AM – 5.30PM:
Instructors: Maciej Swat, Jim Sluka, Xiao Fu, Gui Oliveira, Andy Somogyi
9.00 – 10.30: *CC3D-Hands-on Exercises*
10.30 – 11.00: *Break*
11.00 – 12.30: *CompuCell3D (Fields, Basic Diffusion-based PDEs, Chemotaxis, Hands-on Tutorials)*

12.30 – 1.30: *Lunch*
1:30 – 2:15: *Participants' talks*
2:15 – 3:30: *CompuCell3D (continue Hands-on Tutorial)*
3:30 – 4.00: *Break*
4.00 – 5.30: *CompuCell3D (Advanced Python Scripting in CC3D –Attaching Extra Cell Attributes, Mitosis-Based Simulations, Cell Shape Constraints etc… ,Hands-on Tutorials)*

August 14th , 2014 (Friday)
Day 5: Course: 9AM – 3.30PM:
Instructors: Maciej Swat, Jim, Sluka, Xiao Fu, Gui Oliveira, Andy Somogyi
9.00 – 10.30: *CompuCell3D (continue Advanced Python Scripting in CC3D –Attaching Extra Cell Attributes, Mitosis-Based Simulations, Cell Shape Constraints etc… ,Hands-on Tutorials)*
10.30 – 11.00: *Break*
11:00 – 12:30: *CompuCell3D (continue Hands-on Tutorial)*
12.30 – 1.30: *Lunch*
1:30 – 2:15: *Participants' talks*
2.15 – 3.30: *CompuCell3D (Advanced Python Scripting in CC3D Part 2 – using third party modules in Python, File operations, Post Processing, Simulation Steering – changing CC3DML on-the-fly)*
3.30 – 4.00: *Break*
4.00 – 5.30: *CompuCell3D (Plots and Graphs, configuring CC3D GUI from Python/XML, continue Hands-on Tutorial)*

7.00 – 9.30: ***Hackathon:*** *Building large-scale, predictive/translational tissue models.*

August 15th , 2014 (Saturday)
Day 6: Course: 9AM – 5.30PM:
Instructors: Maciej Swat, Jim, Sluka, Xiao Fu, Gui Oliveira, Andy Somogyi
9.00 – 10.30: *CompuCell3D (SBML-Based Models in CC3D – Reaction Kinetics, ODE, PBPK models, Hands On Tutorials)*
10.30 – 11.00: *Break*
11:00 – 12:30: *CompuCell3D (continue Hands-on Tutorial)*
12.30 – 1.30: *Lunch*
1:30 – 2:15: *Participants' talks.*
2.15 – 3.30: *CompuCell3D (Developing CC3D extension modules in C++ using Twedit++ - demo, Questions-And-Answers session – Suggestions For Future CC3D improvements)*