

**Sub-cellular and Multicellular Modeling Workshop  
at The Hamner Institutes for Health Sciences  
Research Triangle Park, NC USA**

**Instructors: Herbert M. Sauro (Univ. Washington),  
Maciej Swat, James Glazier, Julio Belmonte, 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 10<sup>th</sup>, 2014 (Sunday)*

**Introduction to Python Programming (optional):**

**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 11<sup>th</sup>, 2014 (Monday)*

**Day 1: Course: 9AM – 6.00PM:**

**9.00 – 9.10:** *Welcome note (Jim Sluka, Indiana Univ.)*

**9.10 – 9.20:** *Welcome note (Sudin Bhattacharya, The Hamner Institute)*

**9.20 – 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 12<sup>th</sup>, 2014 (Tuesday)*

**Day 2: Course: 9AM – 5.30PM:**

**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 13<sup>th</sup>, 2014 (Wednesday)*

**Day3: Course: 9AM – 5.30PM:**

**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 - Maciej Swat, Indiana Univ.)*

*August 14<sup>th</sup>, 2014 (Thursday)*

**Day 4: Course: 9AM – 5.30PM:**

**9.00 – 10.30:** *CC3D-Hands-on Exercises – (Maciej Swat, Indiana Univ.)*

**10.30 – 11.00:** *Break*

**11.00 – 12.30:** *CompuCell3D (Fields, Basic Diffusion-based PDEs, Chemotaxis, Hands-on Tutorials - Maciej Swat, Indiana Univ.)*

**12.30 – 1.30:** Lunch

**1:30 – 2:15:** Invited talk- Tom Knudsen EPA

**2:15 – 3:30:** CompuCell3D (continue Hands-on Tutorial - Maciej Swat, Indiana Univ.)

**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 - Maciej Swat, Indiana Univ.)

August 15<sup>th</sup> , 2014 (Friday)

**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 - Maciej Swat, Indiana Univ.)

**10.30 – 11.00:** Break

**11:00 – 12:30:** CompuCell3D (continue Hands-on Tutorial - Maciej Swat, Indiana Univ.)

**12.30 – 1.30:** Lunch

**1:30 – 2:15:** Invited talk- Imran Shah EPA

**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 - Maciej Swat, Indiana Univ. )

**3.30 – 4.00:** Break

**4.00 – 5.30:** CompuCell3D (Plots and Graphs, configuring CC3D GUI from Python/XML, continue Hands-on Tutorial - Maciej Swat, Indiana Univ.)

**7.00 – 9.30: Hackathon:** Combining a PBPK (as SBML) whole body, CompuCell3D multi-cellular and sub-cellular metabolic modeling (SBML) to create a multi-scale model of Acetaminophen (Paracetamol) liver toxicity and therapeutic effects. (CC3D group and The Hamner group but everyone is invited.)

August 16<sup>th</sup> , 2014 (Saturday)

**Day 5: Course: 9AM – 3.30PM:**

**9.00 – 10.30:** CompuCell3D (SBML-Based Models in CC3D – Reaction Kinetics, ODE, PBPK models, Hands On Tutorials – Julio Belmonte, Indiana Univ. )

**10.30 – 11.00:** Break

**11:00 – 12:30:** CompuCell3D (continue Hands-on Tutorial - Julio Belmonte, Indiana Univ.)

**12.30 – 1.30:** Lunch

**1:30 – 2:15:** Invited talk- Dr. Jeff Woodhead, The Hamner.

Title: "The DILIsym Model and its Application to Hepatotoxicity Testing in Drug Development."  
(It will include their work on APAP toxicity modeling.)

**2.15 – 3.30:** CompuCell3D (Developing CC3D extension modules in C++ using Twedit++ - demo, Questions-And-Answers session – Suggestions For Future CC3D improvements - Maciej Swat, James Glazier, Jim Sluka, Julio Belmonte, Indiana Univ.)