# Computational Biology Workshop

August 15th-18th

Hosted by

Howard University and Boston University

| Time | Session Topics | Length |
|---|---|---|
| **Monday, August 15th** | | |
| 9:00 | **Welcome**<br>Refreshments<br>Participant introductions<br>Overview of workshop:<br>Outline, Resources/Handouts | 45’ |
| 9:45 | **Computational biology:**<br>biological models and computational approaches | 45’ |
| 10:30 | **Break** | 15’ |
| 10:45 | **Working with Stella and the Goldbeter model**<br>Intro to cell cycle and numerical modeling<br>Group work: Concept mapping and simulation | 1hr 15’ |
| 12:00 | **Lunch** | |
| 1:00 | **Cell Cycle Models: research papers**<br>Goldbeter, Sha et al., Tyson,<br>Group work: Recognizing components, reactions, testable hypothesis, math | 2hr |
| 3:00 | **Break** | 15’ |
| 3:15 | **Group work: Design and prepare for Tuesday presentation**<br>Sketch initial model of interest<br>Identify related models resources. | 1hr 45’ |

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**Tuesday, August 16th**

| | | |
|---|---|---|
| 9:00 | **Practical and personal considerations in collaborations between experimentalists and theoreticians.**<br>The cell cycle as case: Tyson and Sha et al | 1hr 15 |
| 10:15 | **Break** | 30’ |
| 10:45 | **Designing experiments for numerical modeling**<br>Redesigning data: Exercise | 1hr 15’ |
| 12:00 | **Lunch** | |
| 1:00 | **Group work time**<br>Prepare for group presentation on initial model<br>Investigate potential tools or topics | 1hr 30’ |
| 3:00 | **Break** | |
| 3:15 | **Participant presentations**<br>**Five minutes** | 45’ |
| 4:15 | **Overview of tools** | 45’ |

Wednesday, **August 17th**

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|---|---|---|
| 9:00 | **Reaction Models in Biology**<br>Signal cascades and other biological systems | 45’ |
| 9:45 | **Introduction to JDesigner**<br>Exercises in creating simple reaction models | 45’ |
| 10:30 | **Break** | |

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| Wednesday, **August 17th** | | |
| 10:45 | **Important considerations in constructing models:**<br>Conservation analysis and scales | 1hr 15’ |
| 12:00 | **Lunch** | |
| 1:00 | **Project exercises:**<br>Stochastic models in excel<br>Starting your own | 2hrs |
| 3:00 | **Break** | |
| 3:15 | **Interrogating your model**: Methods of analysis<br>Bifurcation, frequency analysis and metabolic control analysis | 1hr 30’ |
| 4:45 | **Group discussion** | |
| **Thurs** | **August 18th** | |
| 9:00 | **Review of calcium dynamics and studies using Virtual Cell** | 45’ |
| 9:45 | **Introduction to Virtual Cell** | 45’ |
| 10:30 | **Break** | 15 |
| 10:45 | **Hands on with Virtual Cell:**<br>Existing models in database | 1hr 15’ |
| 12:00 | **Lunch** | |
| 1:00 | **Implementing your own model in Virtual Cell** | 2hrs |
| 3:00 | **Break** | 15’ |
| 3:15 | **Work time and wrap up** | 1hr 45’ |