

Computational Modeling Challenge

Overview of the Event

The objective of the computational modeling challenge is to build and test a model of drug dosage and use the model to derive insights on the system behavior with respect to a set of proposed problems. Teams will need to complete a number of activities to successfully complete the event:

1. Review and understand the underlying system concepts and the mathematical representations of the system that are in the provided materials.
2. Alter the Python starting code to complete the model as presented.
3. Verify that the code is providing the correct results within the bounds of the system being modeled.
4. Use the code to test the model sensitivity to selected parameters, to forecast the results through a range of prescribed conditions, and to assemble the appropriate tabular and graphics information to create a summary report.
5. Prepare a summary report describing all of the testing and model outcomes.

In addition to these requirements bonus points will be awarded to the teams that undertake one or more of these activities:

1. Validation of the model against experimental data and/or available literature on the system being modeled.
2. Enhancement of the model by relaxing one or more of the modeling assumptions by adding additional components to the model, conducting the necessary runs, and adding to the summary report.
3. Adding interactive components to the program that allows data input from the keyboard or a file, writes outputs to files, and/or automatically summarizes or compares multiple runs.

Each of the projects is contained in a folder *****on the USB drive you were given (or in an accessible shared folder)*****. In this folder you will find:

1. An overview description of the project presenting the nature of the problem and the available starting materials for the project. This document also specifies the nature of the simulation runs you will need to make once the model is in place.
2. One or more references/articles describing the system and how it has been modeled by others.
3. A starting set of Python code with embedded comments indicating what components you will need to add.
4. Detailed instructions on the format and contents of the final report.
5. Instructions and suggestions for adding bonus options to your model.

Everyone should review the overview document, background materials, and the Python starting code. You should then discuss the approach you will take to creating and testing the initial model. **It is critical to complete this design step before you start working on the code.** You may want to develop a program flowchart, a summary of the mathematical calculations that need to be made, and a list of input requirements and desired outputs to guide your programming tasks.

Once you have completed the design phase, you can divide the subsequent work with one or two people working on parts of the code, one or two gathering any additional data or resources that are needed, one looking ahead to information needed for bonus additions, etc.

Event staff will be available to answer clarification questions about the projects and basic technical questions.