

Development of Interactive Coding Tutorials for Introducing Computational Systems Biology

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Project Overview

Computational systems biology (CSB) has become an increasingly important topic across chemical engineering, biomedical engineering, and biological sciences curricula. However, many students encounter significant barriers when learning CSB concepts due to the mathematical and computational complexity of the field and the limited availability of accessible educational tools for exploring computational models.

This project developed a series of **interactive coding tutorials for computational systems biology** using the **R Shiny** and **learnr** frameworks. The tutorials were designed to help students learn modeling concepts through guided computational exercises, interactive visualizations, and hands-on coding activities.

The work expanded an existing collection of open-access teaching resources previously developed by Dr. Kieslich that introduce computational systems biology concepts using the **R statistical programming language**, which can be found at:

<https://cakieslich.github.io/introCSB/>

These original materials included R Markdown notebooks, interactive Shiny demonstrations, and HTML-based learning modules. The project transformed selected coding examples from those materials into **fully interactive tutorials** that guide students step-by-step through the implementation and analysis of computational models.

Educational Objectives

The primary objective of this project was to lower barriers for students learning computational modeling in systems biology by creating accessible, browser-based instructional tools. The tutorials were designed to:

- Introduce students to modeling biological systems using the R programming language.
- Reinforce conceptual understanding of systems biology models through guided exercises including building systems diagrams and defining systems equations.
- Enable students to simulate and analyze dynamic biological systems.

- Provide instructors with flexible teaching resources that can be integrated into courses in chemical engineering, systems biology, and computational biology.

The tutorials emphasize **active learning**, allowing students to modify code, explore model parameters, and immediately visualize how those changes affect system behavior.

Development of Interactive Tutorials

Interactive tutorials were developed using the **learnr package**, which enables the creation of R-based tutorials with embedded coding exercises, conceptual questions, and automated feedback. The tutorials were deployed through **R shiny**, allowing them to run entirely within a web browser without requiring students to install software.

The resulting modules guide students through core modeling concepts in computational systems biology. Major tutorial topics include:

- Construction of system diagrams for biological models using the `DiagrammeR` package and `Graphviz`.
- Representation of biological systems as networks and directed graphs.
- Implementation and simulation of compartmental models, using **SIR epidemiological models** as the core example.
- Solving systems of ordinary differential equations using the `deSolve` package.
- Visualization and interpretation of model dynamics through time-series plots.
- Extensions of basic models to include additional biological processes (e.g., quarantine compartments).

Through a sequence of guided exercises, students learn how to:

- Translate biological processes into mathematical models.
- Implement models in R code.
- Perform numerical simulations of dynamic systems.
- Analyze and interpret model outputs.

The tutorials combine conceptual explanations, coding tasks, and automated assessments to create a structured learning experience that reinforces both modeling concepts and computational skills.

Implementation and Student Use

The interactive tutorials were developed by the principal investigator in collaboration with a graduate student, Mohammadreza Fahkraei. Dr. Kieslich led the design of the tutorial content and provided training on the use of R Shiny and learnr, while the graduate student assisted in translating existing R coding examples into interactive tutorial formats.

The completed tutorials were integrated into a graduate-level course on **Computational Systems Biology** taught at Auburn University. Within the course, the tutorials were used both as in-class demonstrations and as guided exercises for students to complete independently. The interactive format enabled students with limited prior programming experience to engage with computational modeling concepts and gain confidence working with R-based modeling tools.

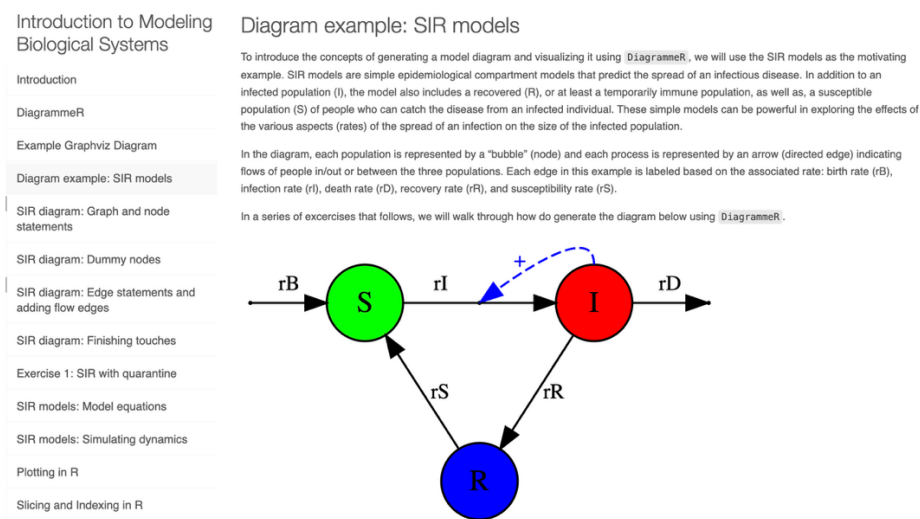


Figure 1. Screenshot of the developed tutorial

Deliverables and Dissemination

The project produced an **open-access interactive tutorial** that is publicly available online. The developed resources include:

- Live interactive tutorials hosted through **shinyapps.io** located at: https://kieslich.shinyapps.io/intro_modeling_tutorial/
- Source code for all tutorials and supporting materials available through a **GitHub repository**

The tutorial and source code are freely available, enabling instructors at other institutions to adopt, adapt, and extend the materials for their own courses. The materials have also been linked through the **CACHE website**, providing broad access to the chemical engineering education community.

Impact

The resources developed through this project provide a modern and accessible platform for teaching computational systems biology concepts. By combining interactive visualization, guided coding exercises, and dynamic simulations, the tutorials allow students to explore complex biological models in a hands-on learning environment.

The browser-based format significantly reduces the technical barriers often associated with computational modeling instruction, making the materials suitable for students from diverse disciplinary backgrounds. In addition, the open-source design of the tutorials ensures that the resources can be expanded and adapted by other instructors.

Overall, this project has produced a set of interactive educational tools that enhance the teaching of computational modeling and support broader integration of systems biology concepts into chemical engineering and related curricula.

Future Directions

The framework developed through this project provides a scalable foundation for additional tutorial development. Future work may expand the library of modules to cover additional modeling topics and explore the development of similar interactive tutorials using **Python-based computational tools**, further broadening accessibility for students and instructors.