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Compartmental Modeling for the Neophyte: An Application of Berkeley Madonna

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Abstract

Compartmental modeling serves as a necessary framework in many fields, especially biomathematics and ecology. This article introduces readers to a user-friendly approach to constructing compartmental models and solving the resulting systems of differential equations to simulate real-world applications. The platform used is Berkeley Madonna, a software package that has an intuitive graphical interface which empowers users—even those with limited mathematical and programming backgrounds—to focus on modeling concepts rather than mathematical or programming intricacies. This makes Berkeley Madonna an ideal platform for students, educators, and researchers.

Keywords: Compartmental Models, Berkeley Madonna, SIR Model, Predator-Prey Model

1 Introduction

The focus of this article is on providing a quick illustration of the ease with which the differential equations solver *Berkeley Madonna* [10] can be used to create and solve a *compartmental model*. With this platform, one can simulate many scenarios by creating and numerically solving a variety of such models *without* having an in-depth knowledge of systems of differential equations, numerical methods, or coding. In fact, as of writing this article, the co-author who developed the examples in Sections 4 and 5 had no formal coursework in programming, modeling, or differential equations.

2 Compartmental Models

Let $X_1, X_2, \ldots, X_n$ represent time-dependent variables and let F_1, F_2, $\ldots$, F_n be functions of $X_1, X_2, \ldots, X_n$, each of which may also include one or more parameters. Then, in *certain* scenarios, a system of first order differential equations of the form shown in the System 1 is referred to as a *compartmental model*.

In mathematical biology, the variables $X_1, X_2, \ldots, X_n$ may represent the sizes of different populations or sizes of subsections of a given population determined by some characteristic of interest at a given time. Each variable can then be thought of as representing a *compartment* in the system under study. The derivatives on the left side of System 1 represent the rates of change with respect to time of the quantities within each compartment.

$$\begin{aligned} \frac{dX_1}{dt} &= F_1(X_1, X_2, \ldots, X_n), \\ \frac{dX_2}{dt} &= F_2(X_1, X_2, \ldots, X_n), \\ &\vdots \\ \frac{dX_n}{dt} &= F_n(X_1, X_2, \ldots, X_n). \end{aligned} \tag{1}$$

How the functions $F_1, F_2, \ldots, F_n$ in a compartmental model are defined is important, as these describe the mechanisms that drive changes in the system under study. It is in constructing the functions $F_1, F_2, \ldots, F_n$ that Berkeley Madonna shines for the novice modeler.

3 Berkeley Madonna

As described on its website [2],

> Berkeley Madonna is an incredibly fast, general purpose differential equations solver. Its graphical interface provides an intuitive platform for constructing complex mathematical models with ease using symbols rather than writing equations. The software provides a suite of graphical tools for plotting your results.

So, Berkeley Madonna has the potential to be an incredibly useful tool for newcomers to the field of mathematical

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modeling in a wide range of areas involving, for example, biological, chemical, ecological, and physical systems.

Go to the Berkeley Madonna website [2] for instructions on downloading and installing the Berkeley Madonna platform, and much more. When Berkeley Madonna is started up, a blank gray screen titled Berkeley Madonna opens up with a menu-bar at the top.

For purposes of this article, of interest at this point is creating a new flowchart through the `File` menu-item to begin the process of constructing a compartmental model (see Figure 1). The next two items in the main menu-bar that will be of use are `Graph` (see Figure 2) and `Parameters` (see Figure 3). Under `Graph`, the options that will be of interest for this article are `Choose Variables` and `Axis Settings`. Also for purposes of this article, the options of interest under `Parameters` are `Define Sliders`, `Show Sliders`, and `Detach Sliders`, with an emphasis on the first.

To get started, click on the `New Flowchart Document` option under `File` in the main-menu. This opens a blank flowchart (see Figure 4) and it is in this window that models will be constructed for the examples in Sections 4 and 5. Before continuing, hover the cursor over each of the yellow icons in the menu-bar at the top of the flowchart window to see what each icon is named. For the time being, four of these are of interest: `reservoir` (), `arc` (), `flow` (), and `global` (). Explanations of how these four tools are used in the flowchart window appear in the first of the examples to follow.

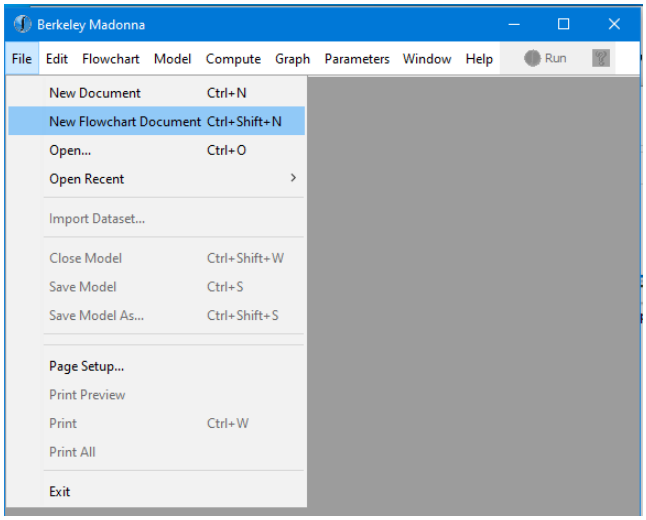

Figure 1: Creating a new flowchart within the `File` menu.

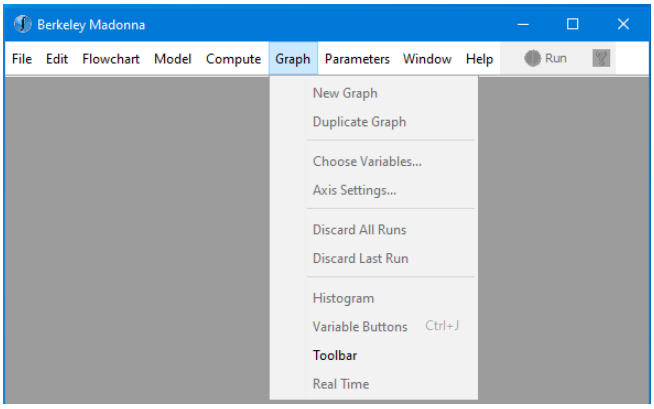

Figure 2: Options within the `Graph` menu-item.

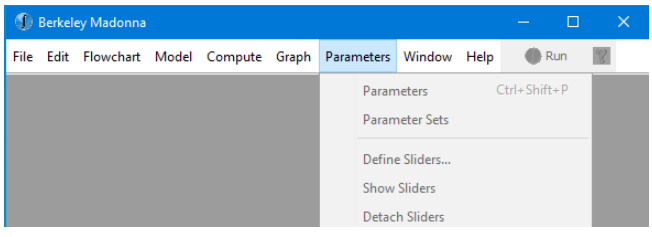

Figure 3: Options within the `Parameters` menu-item.

4 An Infectious-Disease Model

For infectious-disease models, the variables representing the compartments are referred to as *state variables*—they explain a system in *equilibrium*. These state variables all have the same dimensions and typically represent sizes of subsections of a given population at a given time, each subsection being determined by some characteristic of interest. The nature of the system being modeled requires that members of the population move from one subsection to the next. Consider, for example, the *SIR model* for the spread of an infectious disease.

SIR is an acronym for *Susceptible–Infected–Recovered*, and the model described here is the basic model used to introduce modeling the spread of communicable diseases. The compartments in this scenario are identified as being those subsections of a population of interest that include individuals (S) who are susceptible to the disease in question, (I) who have become infected, and (R) who have recovered from the disease.

The underlying mechanics for this model can be described by quantifying the rate (per unit time) at which individuals move into, or out of, each of the three com-

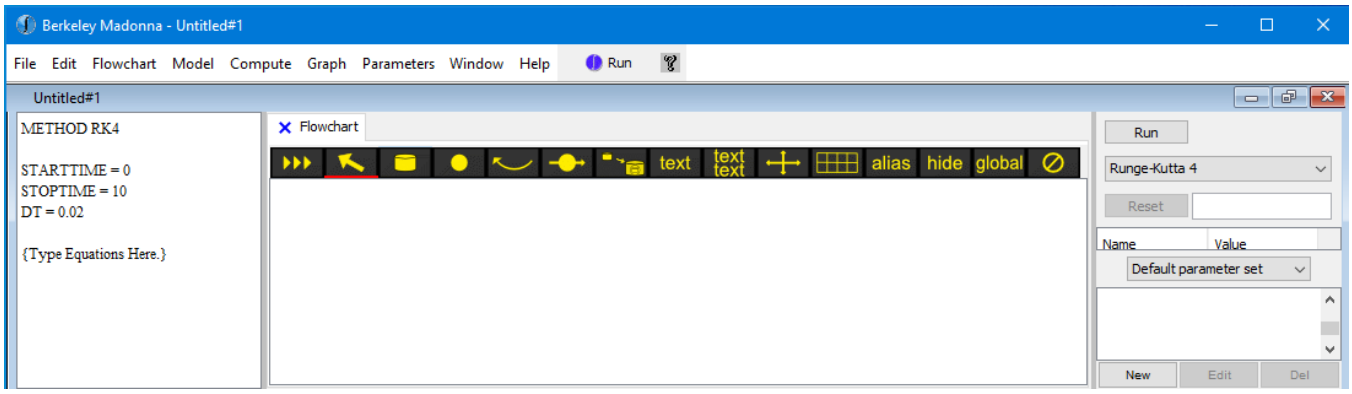

Figure 4: A blank flowchart displaying the model construction buttons of interest and more.

partments. For a population of size N, denote the proportion of individuals in this population who are susceptible to the disease, who have become infected, and who have recovered by S, I, and R, respectively.

Now consider modeling the spread of the Hong Kong Flu in the city of Chicago, which has a population of $N = 2.7$ million people. Suppose the starting number of infected individuals is 10, with the remaining population being classified as susceptible. Also, assume there are no people in the recovered group to start with. The task at hand, then, is to model the flow of individuals from one compartment to the next.

In a Berkeley Madonna flowchart, *reservoirs* represent compartments, and *flows* provide the direction in which members from each compartment move, see Figures 5 and 6 for how these are created. Then, initial values for each compartment are assigned by double-clicking on the "?" symbol on each reservoir and entering the initial values for each—for this example, use $S_0 = 26999990/27000000$, $I_0 = 10/27000000$, and $R_0 = 0$, see Figure 7. Once this is done, notice in Figure 8 that the "?" symbols on the reservoirs have gone away.

Now assume that the population is in equilibrium ($S + I + R = 1$); that instantaneous mixing of the population occurs; that susceptible individuals who come in contact with an infected individual become infected at some constant rate per unit time; and that infected individuals recover at some constant rate per unit time. Under these assumptions, the next task is to define the flows from one reservoir to the next. Let $\alpha = 0.5$ denote the *transmission rate* per unit time of the disease for *each* interaction a susceptible individual has with an infected individual. Since the product SI represents the proportion of interactions between the susceptible and infected individuals—and because of instantaneous mixing—it can be reasoned that at any given time the proportion of susceptible individuals will decrease through infections by the quantity αSI per unit time. Note that under the cur-

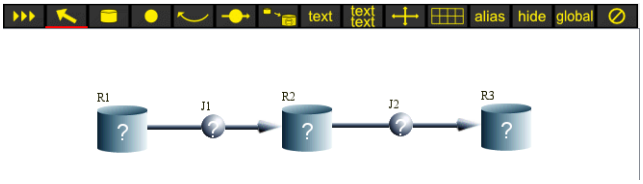

Figure 5: First insert the reservoirs by dragging three of them onto the flowchart sheet. Then insert flows from the first to the second reservoir, and the second to the third.

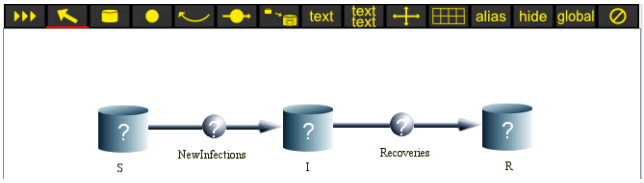

Figure 6: Rename the reservoirs and flows one by one by double-clicking on the existing names and then entering the new names in the text dialog windows that pop up. Once this is done, move the names by dragging them to desired locations.

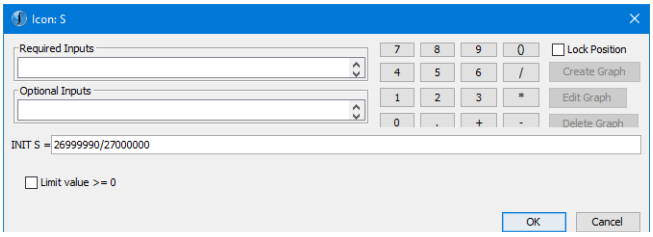

Figure 7: Double-click on the S reservoir to open the S-icon window, then enter the initial value for the susceptible population (as a proportion of 2.7 million). Repeat the process for the I and R reservoirs.

rent setup, the parameter α has units time^{-1} since the proportions S and I are dimensionless.

Next, let $\beta = 0.33$ denote the *recovery rate* per unit time of an infected individual. Then, at any given time the rate at which the proportion of recovered individuals increases per unit time will be βI. The parameter β also has units time^{-1} since I is dimensionless.

Finally, at any given time, the rate at which the proportion of infected individuals changes per unit time is found by subtracting the proportion of individuals who recover from the proportion who get infected.

The first step in defining the flows is to provide access to the parameter values α and β. This is done by clicking on the `global` button on the flowchart menu-bar and then entering the values, see Figures 8 and 9. Next, go back to the flowchart window and insert the relevant arcs from the reservoirs to the respective flow buttons by clicking on the `arc` button in the flowchart menu-bar and then dragging an arc from, for example, the S reservoir *onto* the flow button out of the S reservoir, see Figure 10. Finally, double-click on the flow buttons and enter the appropriate computational formulas, see Figures 11 and 12.

Once all of this has been done, save the completed SIR model flowchart. Figure 13 provides a complete picture of what appears on this flowchart. On careful examination it will be noticed that the panel on the left provides details of the model itself, that is, a specific case of the generic SIR model:

$$\frac{dS}{dt} = -\alpha SI, \qquad \frac{dI}{dt} = \alpha SI - \beta I, \qquad \frac{dR}{dt} = \beta I, \qquad (2)$$

with initial values being denoted by $S(0) = S_0$, $I(0) = I_0$, and $R(0) = R_0$.

The panel on the right provides relevant settings for the numeric solution of the defined system of equations. Before proceeding to the solution of this system, click on `STOPTIME` in the panel on the right and set this to 150 (*do not* click on the `Reset` button), similarly set the time-step `DT` to 0.01. Then, click on the `Run` button to solve the system and obtain the solution curves, see Figure 14. It should be noted that the vertical scale for the infected curve, I, indicated on the vertical axis on the right is different from the vertical scale for susceptible and recovered curves. Axis settings can be changed, if so desired, by clicking on the `Graph` button in the main menu-bar and selecting `Axis Settings` to change the default settings.

To include an additional useful feature on this graph, click on the `Parameters` button on the main menu-bar and select the `Define Sliders` option. In the `Define Sliders` pop-up window, see Figure 15, click on and add the parameter `alpha`, setting the minimum to 0 and the maximum to 1. Similarly, click on and add the `beta` parameter and set its range from 0 to 1. The result is displayed in Figure 16.

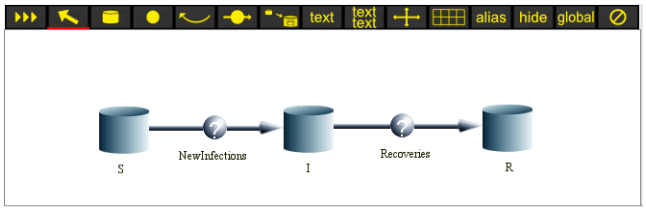

Figure 8: The flowchart appearance once the initial values for S, I, and R have been entered.

Figure 9: Enter parameter values as global quantities.

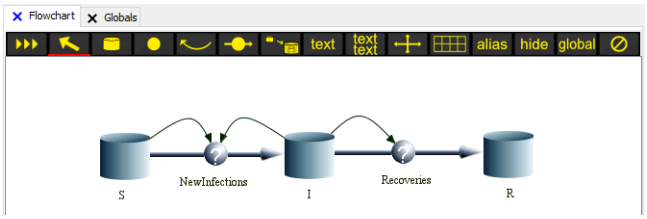

Figure 10: Since the proportion of new infections is quantified by αSI, insert arcs from the S and I reservoirs to the flow out of the S reservoir. Since the proportion of recoveries is quantified by βI, insert an arc from the I reservoir to the flow out of the I reservoir.

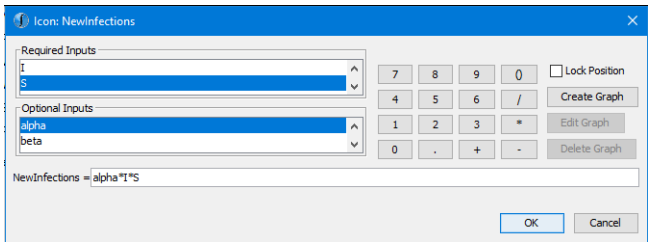

Figure 11: The proportion of new infections is αSI.

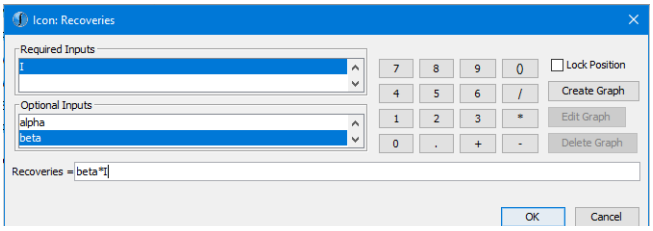

Figure 12: The proportion of recoveries is βI.

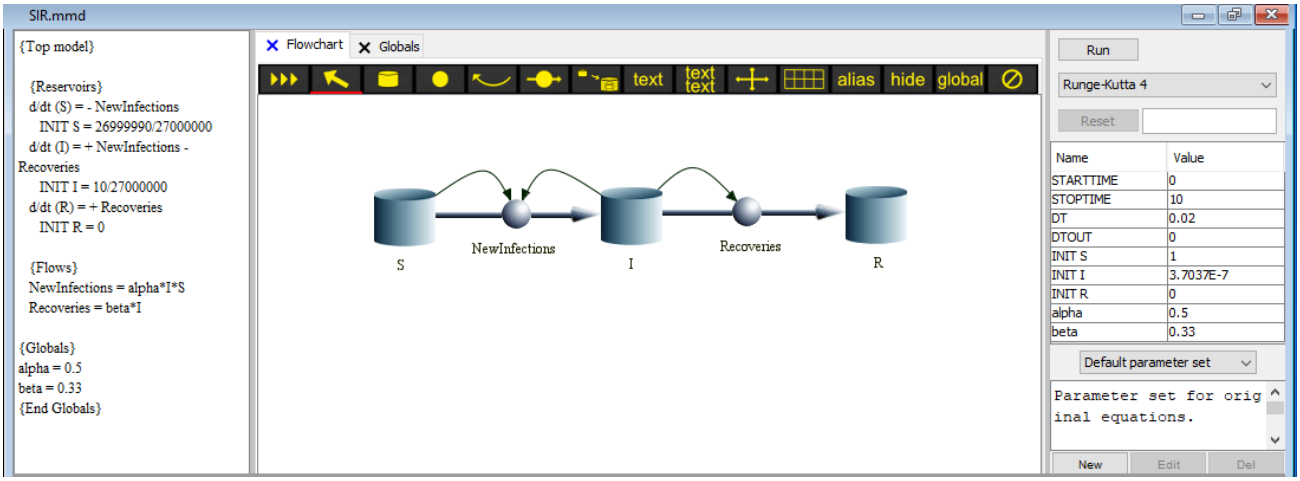

Figure 13: The completed flowchart for the SIR model.

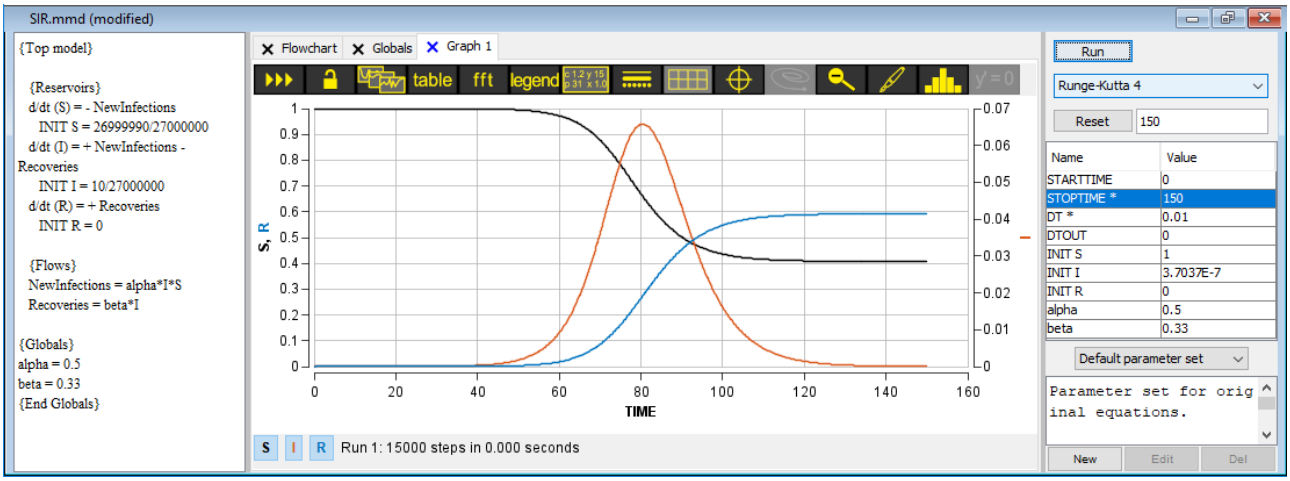

Figure 14: Solution curves for the SIR model.

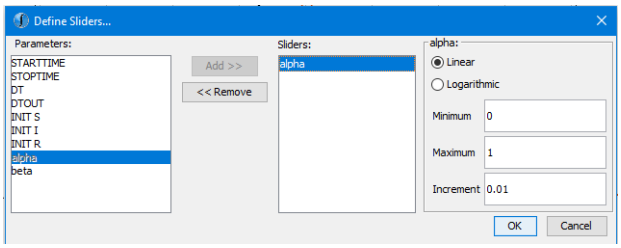

Figure 15: Defining and inserting parameter sliders.

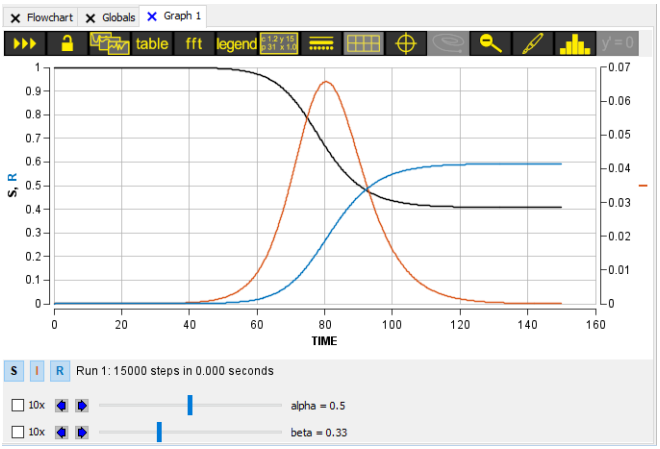

Figure 16: Graphs of the solution curves with sliders.

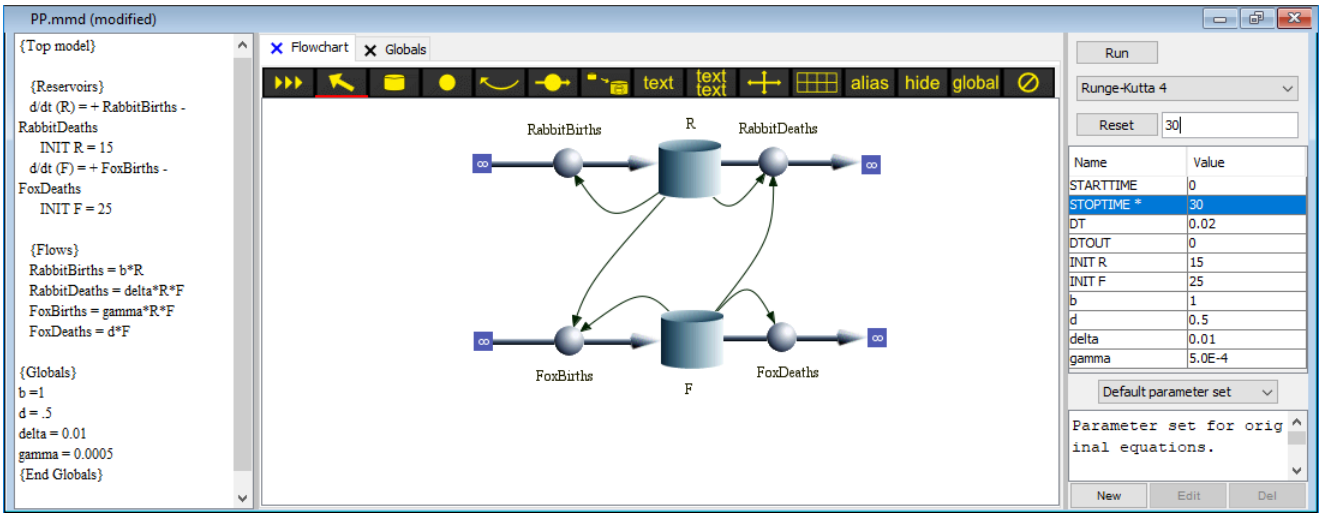

Figure 17: The completed flowchart for the rabbit-fox predator-prey model.

It is now possible to explore the dynamics of the epidemic by moving the sliders back and forth. To do this, drag the sliders or click on the blue arrows to the left of the sliders. Note that it is very likely that the `STOPTIME` will have to be adjusted with changes to the parameter values—a `STOPTIME` slider would be useful for this.

Note that the range (`Minimum` and `Maximum`) for sliders does not need to be $[0, 1]$, choose a range that best suits the scenario under study. Also, once sliders are defined and inserted in a graph they can be hidden (or detached) by selecting `Hide Sliders` (or `Detach Sliders`) in the `Parameters` main-menu. Or they can be reinserted by selecting `Show Sliders` (or `Reattach Sliders`) in the `Parameters` main-menu.

Having constructed the model and set the stage for solutions/simulations, it becomes possible to perform relevant desired analyses of the epidemic under study. The formal analyses stage is beyond the scope of this article, so the interested reader is referred to, for example, [4] for an elementary development of this model, and [5] or [8, Sec. 6.6] for deeper treatments.

5 A Predator-Prey Model

For this example, consider modeling the population sizes of a prey species, say rabbits, and its sole predator species, say foxes, in a closed ecosystem. Let R and F denote the sizes of these two populations, respectively. Then, unlike for the SIR model, in the context of a *predator-prey model* the variables do not describe a system in equilibrium, that is, the sum total of the prey and predator populations does not remain constant. Regardless, each species does represent a compartment in the system. In addition to instantaneous mixing of the two populations, some further assumptions are made here.

It is assumed that increases in the prey population size per unit time occur through births, which are influenced by the availability of food and which are assumed to outpace natural mortality (in the absence of predation). Then, net decreases in the prey population size can be viewed as occurring soley through predation. Conversely, it is assumed that increases in the predator population size per unit time occur through births, which are also influenced by the availability of food (the prey), and in this case net decreases in the predator population size are assumed to occur through natural mortality (which includes deaths through starvation).

Let b denote the birth rate for the prey. Then, the prey population size will increase by the quantity bR per unit time. Denote the rate at which each predator-prey interaction results in a prey death by δ. Then the decrease in the prey population size per unit time as a result of predation will be δRF. Next, let d denote the death rate for the predator. Then the decrease in the predator population size per unit time will be dF. Finally, denoting the rate of growth in the predator population size due to the effect of each interaction with a prey by γ, the predator population size increase per unit time will be γRF. Observe that the units for the parameters b and d are time^{-1}, and the units for δ and γ are $(\text{counts}\times\text{time})^{-1}$.

This information can then be used to construct a flowchart that describes the predator-prey system in question. There is one important point to note for this system. Unlike in the previous example, individuals from the two populations (compartments) R and F do not move from one to the other. This means that *flows* between the two *reservoirs* are not drawn. However, interactions between the two do occur, and so *arcs* defining a flow may come

from both reservoirs.

For purposes of this example, consider starting with the parameter values[1] $b = 1$, $d = 0.5$, $\delta = 0.01$, and $\gamma = 0.0005$, and consider initial populations of $R_0 = 15$ and $F_0 = 25$. Then, following the process described for creating a flowchart in the previous example, the flowchart describing this particular predator-prey system takes on the appearance of Figure 17.

As before, the panel on the left in Figure 17 gives details of the system being modeled, which corresponds to the general form

$$\frac{dR}{dt} = bR - \delta RF, \qquad \frac{dF}{dt} = -dF + \gamma RF, \qquad (3)$$

with initial conditions being denoted by $R(0) = R_0$ and $F(0) = F_0$. This system of equations, called the Lotka-Volterra equations, serves as a popular first example of modeling predator-prey systems.

Now, using a `STOPTIME` of 30, click on the `Run` button to get graphs of the solution curves. Then, in the `Axis Settings` pop-up from the `Graph` main-menu, deselect the `auto` scaling boxes for the left and right vertical axes and make them the same, see Figure 18 for the end result.

Another useful plot for this system is the plot of the predator population size against the prey population size (F against R). To get this graph, select `New Graph` from `Graph` in the main-menu, and then with the `Graph 2` window activated, select `Choose Variables` from the `Graph` main-menu. Then, in the pop-up window, place R in the `X-Axis` and F in the `Y-Axis`. Click on `OK` and then click on `Run` again. The resulting graph, see Figure 19, reveals that the population-size pairs follow a cyclic curve.

Here is another nice feature. In the `Graph 2` window, hover the cursor over the menu-bar above the graph to see the names of the menu-buttons. There are two buttons of interest, `Overlay Plots` and `Initial Conditions`. Click on both of these menu-items and then hover the cursor over the graph. Notice that the cursor takes on the appearance of cross-hairs. Pick a location on the axes and click the mouse. The new overlayed graph, see Figure 20, represents the graph of a system with initial conditions corresponding to the point on the axes where the mouse was clicked, see the lower-left corner of Figure 20.

Just as shown for the previous example, sliders can be attached to, or detached from, either of the graphs constructed (be sure to deselect the `Overlay Plots` and `Initial Conditions` buttons). These sliders can then be used to explore the effects of adjusting parameter values of interest.

Again, deeper formal analyses of such models are beyond the scope of this article. See, for example, [6,

[1]See https://mathinsight.org/introducing_rabbit_predators

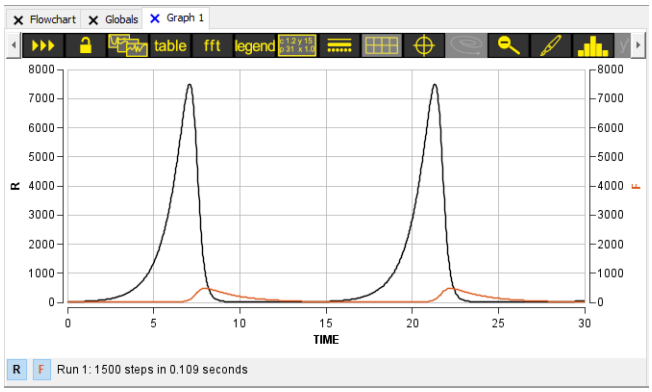

Figure 18: Solution curves for the rabbit and fox populations against time.

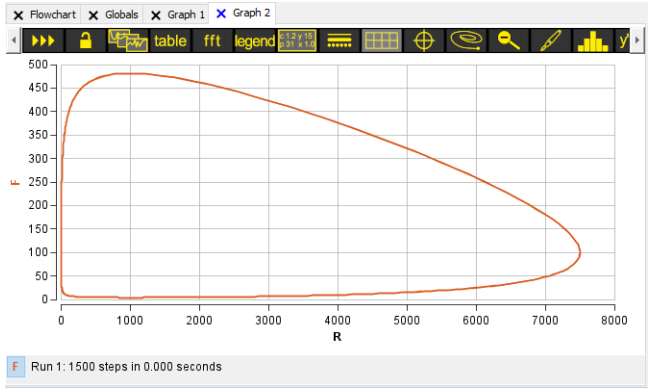

Figure 19: Plot of fox populations against rabbit populations. If so desired, sliders for one or more of the parameters can be attached to this plot.

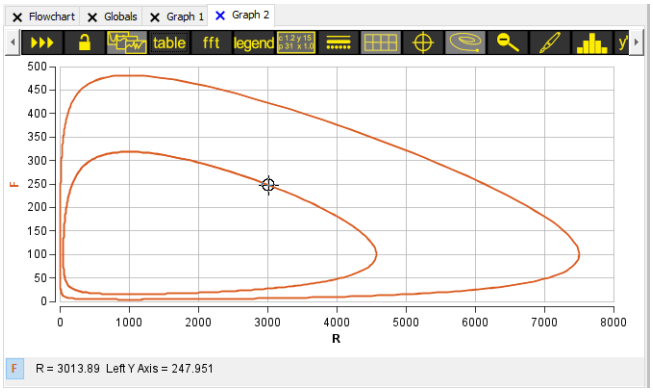

Figure 20: Plots with different initial conditions. The location of the cross-hairs marks the new initial conditions.

Sec. 9.5] or [8, Sec. 6.2] for technical details on the underlying theory and model analyses.

6 Closing Comments

The examples presented in this article were chosen for their relative simplicity so as to provide illustrations of constructing flowcharts for two versions of compartmental models. It is expected that readers may be interested in delving deeper into such applications. There are some additional useful features in Berkeley Madonna that lie within the scope of this article and that can be explored using the examples provided. Readers are encouraged to explore the various capabilities available in the main menu and the various options in the flowchart menu.

A user's guide to Berkeley Madonna is available on the Berkeley Madonna website [2], and examples of using Berkeley Madonna in more complex settings can be found in the tutorials [10] and [11], including importing data sets and fitting data to models. The interested reader can also find further details and directions to resources on the evolution of models in epidemiology in, for example, [1], [3], [7], and [9]. Similarly, details and directions to resources on the evolution of predator-prey models can be found in, for example, [6] and [8].

Acknowledgments

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Author Contributions

The idea of preparing a *Compartmental Modeling for the Neophyte* article was conceived by Olcay Akman at the 2023 CURE workshop of the IBA. Siddharth Bhumpelli and Cody Cline conducted preliminary research into compartmental models and selected the examples presented in this article. Siddharth Bhumpelli then focused on understanding how to use Berkeley Madonna on the examples chosen, while Cody Cline served as a "student sounding board" in the development of accessible instructions on its use. Olcay Akman and Christopher Hay-Jahans served as mentors for this project, providing guidance on focusing efforts, researching the literature, and writing.

References

[1] Allen, L. J., Brauer, F., Van den Driessche, P., & Wu, J. (2008). *Mathematical Epidemiology* (Vol. 1945). Berlin: Springer.

[2] Berkeley Madonna Version 10 (n.d.), https://berkeley-madonna.myshopify.com/

[3] Berryman, A. A. (1992). The origins and evolution of predator-prey theory. *Ecology*, 73(5):1530-1535.

[4] Best, A. (2023). *Introducing Mathematical Biology*. University of Sheffield Pressbooks Network Open Textbook Library, Sheffield, UK. Retrieved August 31, 2023 from https://open.umn.edu/opentextbooks/textbooks/1441.

[5] Blackwood, J. C., & Childs, L. M. (2018) An introduction to compartmental modeling for the budding infectious disease modeler. *Letters in Biomathematics*. 5(1):195–221.

[6] Boyce, W. E. & DiPrima, R. C. (2020). *Elementary Differential Equations and Boundary Value Problems*. Wiley.

[7] Brauer, F., Castillo-Chavez, C., & Feng, Z. (2019). *Mathematical Models in Epidemiology* (Vol. 32). New York: Springer.

[8] Edelstein-Keshet, L. (2005). *Mathematical Models in Biology*. Society for Industrial and Applied Mathematics.

[9] Frantzen, J. (2023). *Epidemiology of Infectious Diseases*. Leiden, The Netherlands: Wageningen Academic.

[10] Marcoline, F. V., Furth, J., Nayak, S., Grabe, M., & Macey, R. I. (2022). Berkeley Madonna Version 10–A simulation package for solving mathematical models. *CPT: Pharmacometrics & Systems Pharmacology*, 11(3), 290-301.

[11] Shiflet, A. B., & Shiflet, G. W. (2014). *Introduction to Computational Science: Modeling and Simulation for the Sciences*. Princeton University Press. Retrieved October 7, 2023 from https://ics.wofford-ecs.org/dynamics/Berkeley-Madonna