Answers to Exercises

Introduction to Computational Science:
Modeling and Simulation for the Sciences, 2nd Edition

Angela B. Shiflet and George W. Shiflet
Wofford College

Chapter 4

Module 4.1

1. **a.** $dW/dt = aW - bWB$, $dB/dt = cB - dWB$, $W_0 = 20$, $B_0 = 15$
b. $a = bB$ and $c = dW$, where b and d are any nonnegative real numbers
Answer correction courtesy of Naiyf S. Alsaud
Ph.D. Candidate in Astrophysics
University of Edinburgh, UK, at the Royal Observatory

2. **a.** One possible model: $dW/dt = (1 - W/M_W)(aW - bWB)$, $dB/dt = (1 - B/M_B)(cB - dWB)$, $W_0 = 20$, $B_0 = 15$, where M_W and M_B are the carrying capacities for the respective populations
b. $a = bB$ and $c = dW$, where b and d are any nonnegative real numbers
Answer correction courtesy of Naiyf S. Alsaud
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University of Edinburgh, UK, at the Royal Observatory

3. **a.** higher
b. lower
c. lower
d. lower

Module 4.2

1. For equilibrium in (1) or (2), $ds/dt = dh/dt = 0$ implies $k_s = hk_{hs} = (3000)k_{hs}$ and $k_h = sk_{sh} = (500)k_{sh}$. One solution: $k_s = 0.6$, $k_{hs} = 0.0002$, $k_h = 0.1$, $k_{sh} = 0.0002$. Another solution: $k_s = 0.9$, $k_{hs} = 0.0003$, $k_h = 0.5$, $k_{sh} = 0.001$ (Correction courtesy of Naiyf S. Alsaud)

2. $\Delta s = k_s * s(t - \Delta t) - k_{hs} * h(t - \Delta t) * s(t - \Delta t)$ and
$\Delta h = k_{sh} * s(t - \Delta t) * h(t - \Delta t) - k_{sh} * s(t - \Delta t) * h(t - \Delta t)^2 / M$
or $ds/dt = k_s s - k_{hs} hs$ and $dh/dt = k_{sh} sh - k_{sh} sh^2 / M$
Alternative model:
$\Delta s = k_s * s(t - \Delta t) - k_{hs} * h(t - \Delta t) * s(t - \Delta t)$ and
$\Delta h = (k_{sh} * s(t - \Delta t) * h(t - \Delta t) - k_{sh} * h(t - \Delta t)) - (h(t - \Delta t) / M) (k_{sh} * s(t - \Delta t) * h(t - \Delta t) - k_{sh} * h(t - \Delta t))$

or $ds/dt = k_s s - k_{hs} hs$ and $dh/dt = (k_{sh} sh - k_{sh} h) - (h / M)(k_{sh} sh - k_{sh} h)$

3. Where s is the number of krill and h is the number of blue whales,
$\Delta s = (k_s * s(t - \Delta t) * (1 - s(t - \Delta t)/M_s) - k_{hs} * h(t - \Delta t) * s(t - \Delta t)) * \Delta t$ and
$\Delta h = k_{sh} * h(t - \Delta t) (1 - h(t - \Delta t) / (k * s(t - \Delta t)))) * \Delta t$, where k is a constant

Module 4.3

1. $dS/dt = -0.0058SI$, $dI/dt = 0.0058SI - 0.04I$, $dR/dt = 0.04I$

2. $dS_Q/dt = qk(1 - b)I_U S/N_0 - uS_Q$

3. $dE/dt = kb(1 - q)I_U S/N_0 - pE$

4. $dE_Q/d\mathrm{t} = qkbI_U S/N_0 - pE_Q$

5. $dS/dt = uS_Q - kb(1 - q)I_U dS/N_0 - qkbI_U S/N_0 - qk(1 - b)I_U S/N_0$

6. $dI_U/dt = pE - wI_U - mI_U - vI_U$

7. $dI_D/dt = wI_U + wI_Q - vI_D - mI_D$

8. $dI_Q/dt = pE_Q - mI_Q - vI_Q - wI_Q$

9. $d\,(recovered\_immune)/dt = vI_D + vI_U + vI_Q$

10. $dD/dt = mI_Q + mI_D + mI_U$

11. **a.** $3^{10} = 59{,}049$
b. all
c. $3^{15} = 14{,}348{,}907$
d. all

Module 4.4

1. Heat, humidity, poverty, lack of mosquito netting, insecticides, remoteness

2. $d(human\_hosts)/dt = (prob\_bit)(prob\_vector)(uninfected\_humans) - (recovery\_rate)(human\_hosts) - (malaria\_induced\_death\_rate)(human\_hosts) - (immunity\_rate)(human\_hosts)$

3. $d(uninfected\_mosquitoes)/dt = (mosquito\_birth\_rate)(mosquitoes) - (prob\_bite\_human)(uninfected\_mosquitoes)(human\_hosts / humans) - (mosquito\_death\_rate)(uninfected\_mosquitoes)$

4. $d(vectors)/dt = (prob\_bite\_human)(uninfected\_mosquitoes)(human\_hosts / humans) - (mosquito\_death\_rate)(vectors)$

Module 4.5

1. $d[\text{E}]/dt = -d[\text{ES}]/dt$

2. $$v = \frac{v_{\max}[\text{S}]}{K_m + [\text{S}]} \approx \frac{v_{\max}K_m}{K_m + K_m} = \frac{v_{\max}}{2}$$

3.
- **a.** $d[\text{E}]/dt = k_3[\text{ES}] - k_1[\text{E}][\text{S}]$
- **b.** $d[\text{ES}]/dt = k_1[\text{E}][\text{S}] -(k_2 + k_3)[\text{ES}]$
- **c.** $d[\text{P}]/dt = k_3[\text{ES}]$
- **d.** $v = d[\text{P}]/dt$
- **e.** $[\text{E}][\text{S}] = (k_3 / k_1)[\text{ES}]$
- **f.** $[\text{E}][\text{S}] = K_m[\text{ES}]$
- **g.** $K_m = [\text{E}][\text{S}] / [\text{ES}]$
- **h.** $[\text{E}] = [\text{E}_0] - [\text{ES}]$
- **i.** $[\text{ES}] = [\text{E}_0][\text{S}] / (K_m + [\text{S}])$
- **j.** $d[\text{P}]/dt = k_3[\text{E}_0][\text{S}] / (K_m + [\text{S}])$
- **k.** $d[\text{P}]/dt$ approaches v_{max} and $k_3[\text{E}_0]$
- **l.** $v = v_{max}[\text{S}] / (K_m + [\text{S}])$

4. $d[\text{ES}]/dt = k_1[\text{E}][\text{S}] - (k_2 + k_3)[\text{ES}]$, which by Assumption 4 (see Exercise 3 h) and the assumption that $d[\text{ES}]/dt \approx 0$, is $d[\text{ES}]/dt = k_1([\text{E}_0] - [\text{ES}])[\text{S}] - (k_2 + k_3)[\text{ES}] \approx 0$. Thus, solving for [ES], we have the approximation $[\text{ES}] = k_1[\text{E}_0][\text{S}]/((k_2 + k_3) + k_1[\text{S}])$. Dividing each term of the numerator and denominator by k_1, we have $[\text{ES}] = [\text{E}_0][\text{S}]/((k_2 + k_3)/k_1 + [\text{S}]) = [\text{E}_0][\text{S}]/(K + [\text{S}])$, where $K = (k_2 + k_3)/k_1$. Thus $d[\text{P}]/dt = k_3[\text{ES}] = k_3[\text{E}_0][\text{S}]/(K + [\text{S}])$.

5. $v = v_{max}[\text{S}] / (K_m + [\text{S}]) \Rightarrow 1/v = (K_m + [\text{S}])/(v_{max}[\text{S}]) = K_m/(v_{max}[\text{S}]) + [\text{S}]/(v_{max}[\text{S}]) \Rightarrow$
$$\frac{1}{v} = \frac{K_m}{v_{\max}}\left(\frac{1}{[S]}\right) + \frac{1}{v_{\max}}$$

6.
- **a.** $d[\text{S}]/dt = -k_1[\text{E}][\text{S}]^n + nk_2[\text{ES}]$
- **b.** $d[\text{E}]/dt = -k_1[\text{E}][\text{S}]^n + k_2[\text{ES}] + k_3[\text{ES}]$
- **c.** $d[\text{P}]/dt = k_3[\text{ES}]$
- **d.** $d[\text{ES}]/dt = k_1[\text{E}][\text{S}]^n - (k_2 + k_3)[\text{ES}] = -d[\text{E}]/dt$

7. $d[\text{P}]/dt = k_3[\text{E}_0][\text{S}]^n / (K_m + [\text{S}]^n) = v_{max}[\text{S}]^n / (K_m + [\text{S}]^n)$