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# Pitfalls and Pluses in Using Numerical Software to Solve Differential Equations

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Abstract: Ordinary differential equations (ODEs) are often used to model the behavior of physical phenomena and textbooks today especially demonstrate this fact. Since only a very small collection of ODEs can be solved analytically, there is often no alternative than to use computer software to gain some insight into the behavior of solutions (and sometimes even if solution formulas are available—the formulas are often complicated!). A classic work on the numerical solution of ODEs was authored by Shampine [\[8\]](#page-16-0).

There are some questions about the behavior of solutions of ODEs that are not quite appropriate for numerical solvers. In this paper we present examples which illustrate some of these features. However, there is no disputing the fact that the output of numerical solvers is often useful for portraying and understanding the behavior of solutions of ODEs and their utility in modeling physical phenomena, as our final example shows.

## 1 Introduction

Numerical ODE solvers use a discrete numerical algorithm to approximate a continuous, piecewise smooth solution and hence one must always ask if an artifact produced by a solver is really present in the solution or just a product of the discretization process that produced the numerical solution. It also is a fact that if parameters in a solver are adjusted then sometimes artifacts arise in the output that were not there before (this is especially true when a driving term in the ODE is piecewise continuous). Finally, results may vary from one numerical solver to another.

Using a numerical solver to produce an approximate solution of an initial value problem (IVP) is not a mindless operation; it is not merely inserting an IVP into a package solver and out pops a decent approximate solution. The papers by Stewart  $[13]$ , Shampine [\[9,](#page-17-1) [10,](#page-17-2) [11,](#page-17-3) [12\]](#page-17-4), and Hubbard [\[6\]](#page-16-1) cite some pitfalls in using numerical ODE solvers and give some cautionary examples in this regard. We give some examples below; other examples can be found in Borrelli and Coleman's "Modeling and Visualization with ODE Architect"  $\lceil 2 \rceil$ .

#### 2 Examples

Example 2.1 (Longer to Rise or to Fall?). Throw a ball straight up in the air. Does it take longer to rise or to fall? Or does it take equal time? The gravitational force acting on the ball is constant while the ball is in the air, but air puts a drag force on the ball. The magnitude of this drag force is proportional to the ball's speed (if the ball is light) and acts in a direction opposite to the ball's motion (this is viscous damping). Nowadays this question could be answered experimentally using sensors and accurate timers in a physics lab. Galileo, on the other hand, would have cut a groove in a frictionless plane and rolled the ball in the groove with the plane only slightly inclined. Another approach might be to perform a thought experiment as follows: Newton says that the force acting on the ball is equal to the ball's mass times its acceleration. The gravitational force acting on the ball is constant in value (near the earth's surface) and always acts downward while the ball is in motion. But the drag force on the ball acts downward when the ball rises and upward when the ball is falling. Hence a larger total force acts on the ball when it rises than when it falls. So the ball accelerates more slowly when it is falling and it takes longer to fall than to rise.

Another approach to answering this question would be to model the motion of the ball with a differential equation and then visually examine the output graph produced by using a numerical ODE solver on the appropriate initial value problem (IVP). This is the approach which was used in Example 1.4.1 of our text  $\lceil 1 \rceil$ . If the ball is thrown upward from ground level with initial velocity  $v_0$ , then using Newton's Second Law the position  $y$  of the ball above the ground at time  $t$  is given by the IVP

<span id="page-2-0"></span>
$$
my'' = -mg - cy', \quad y(0) = 0, \quad y'(0) = v_0 \tag{2.1}
$$

where  $m$  is the mass of the ball,  $q$  is the gravitational constant (and hence  $mg$  is the gravitational force on the ball), and  $cy'$  is the viscous drag on the ball due to the air, where c is the positive drag constant. For this case we could use a grapher because, as we shall soon see, there is a formula for the solutions of IVP  $(2.1)$ . But solution formulas are not always available and then a numerical ODE solver must be used. Our solver/grapher produced the graphs in Figures [1](#page-3-0) and [2](#page-3-1) for various values of  $m$ ,  $c$ , and  $v_0$ 

Inspection of these graphs reveals that the ball takes longer to fall than to rise. But is that the end of the story? Not exactly. Numerical ODE solvers require specific values for the parameters  $m$ , c and  $v_0$ , and we used only a few specific values of the parameters to produce the graphs shown in the figures. From those few values we inferred what would happen for *any* positive values of the parameters. Such an inference is not quite justified. This shows a weakness in using numerical solvers in answering some kinds of questions. Let's try to improve this situation with an analytical solution of IVP  $(2.1)$ . Writing the ODE in the form

<span id="page-2-1"></span>
$$
y'' + \frac{c}{m}y' = -g \tag{2.2}
$$

we see that a particular solution for the driven ODE [\(2.2\)](#page-2-1) is

$$
y_d = -\frac{gm}{c}t\tag{2.3}
$$



<span id="page-3-0"></span>Figure 1: Viscous damping model:  $c/m = 3$  and four initial velocities.



<span id="page-3-1"></span>Figure 2: Viscous damping model with smaller mass  $m : c/m = 10$ .

and that the general solution of the undriven ODE  $y'' + cy'/m = 0$  is

$$
y_u = C_1 e^{-ct/m} + C_2 \tag{2.4}
$$

where  $C_1$  and  $C_2$  are constants. Thus, the general solution for the ODE [\(2.2\)](#page-2-1) is

$$
y_{\text{gen}} = y_u + y_d = C_1 e^{-ct/m} + C_2 - \frac{gm}{c}t \tag{2.5}
$$

where  $C_1$  and  $C_2$  depend on the initial conditions given in IVP [\(2.1\)](#page-2-0). Using the conditions given in  $(2.1)$  we find the solution of IVP  $(2.1)$  to be

<span id="page-4-1"></span>
$$
y = \left(-\frac{gm^2}{c^2} - \frac{m}{c}v_0\right)\left(e^{-ct/m} - 1\right) - \frac{gm}{c}t.
$$
 (2.6)

Now the initial time is  $t_0 = 0$ , so let T be the time the ball reaches the top of its motion and begins to fall toward the ground. Hence,

$$
0 = y'(T) = \left(\frac{gm}{c} + v_0\right)e^{-cT/m} - \frac{gm}{c}
$$
\n
$$
(2.7)
$$

and it follows that

<span id="page-4-0"></span>
$$
e^{cT/m} = 1 + \frac{c}{gm}v_0.
$$
 (2.8)

Using equation [\(2.8\)](#page-4-0) we can rewrite the solution  $y(t)$  in [\(2.6\)](#page-4-1) as

<span id="page-4-2"></span>
$$
y(t) = \frac{gm^2}{c^2} e^{cT/m} \left( 1 - e^{-ct/m} \right) - \frac{gm}{c} t \tag{2.9}
$$

From equation  $(2.9)$  we have that

$$
y(2T) = \frac{gm^2}{c^2} \left( e^{cT/m} - e^{-cT/m} \right) - \frac{gm}{c} 2T
$$

$$
= \frac{2gm^2}{c^2} \left( \frac{e^{cT/m} - e^{-cT/m}}{2} - \frac{cT}{m} \right)
$$

$$
= \frac{2gm^2}{c^2} \left( \sinh \frac{cT}{m} - \frac{cT}{m} \right) > 0
$$

for all possible positive values of m and c, (since sinh  $u > u$  for all  $u > 0$ ). Thus the ball takes longer to fall than to rise no matter what the mass of the ball is or what the positive drag coefficient  $c$  is (provided, of course, that the modeling ODE is still valid).

<span id="page-4-3"></span>Example 2.2 (Predator-Prey Interaction with Constant Effort Harvesting). Suppose that we are dealing with two populations which are undergoing a predator-prey interaction and that, in addition, each population is being harvested at the same proportional rate. Using the Balance Law and the Population Law of Mass Action (see p. 10 and p. 86 in [\[1\]](#page-16-3)), we showed in Section 2.6 of [\[1\]](#page-16-3) that the predator population x and the prey population  $y$ satisfy the differential equations

$$
x' = -ax + bxy - Hx \tag{2.10}
$$

<span id="page-4-4"></span>
$$
y' = cy - dxy - Hy \tag{2.11}
$$



<span id="page-5-1"></span><span id="page-5-0"></span>Figure 3: The effects of harvesting.

where a, b, c, d, and H are positive constants In Example 2.6.2 in[\[1\]](#page-16-3), we considered the special case with initial data,

$$
x' = -x + xy/10 - Hx, \t x(0) = 8 \t (2.12)
$$

$$
y' = y - xy/5 - Hy, \t\t y(0) = 16. \t\t (2.13)
$$

The orbits in state space for IVP  $(2.13)$  were plotted for various values of H and the results are shown in Figure [3.](#page-5-1)

Of course, all of the orbits pass through the point (8, 16) at the initial time  $t_0 = 0$ , but the orbits also appear to pass through another common point. The question is this: is this an artifact of the discrete numerical algorithm which produced the graph or is there indeed another common point on all the orbits of IVP  $(2.13)$  for any value of  $H > 0$  other than the initial point (8, <sup>16</sup>)?

To answer that question we proceed as follows. Since the differential system [\(2.13\)](#page-5-0) is autonomous, we see that all orbits of the system are integral curves of the first order ODE

<span id="page-5-2"></span>
$$
\frac{dy}{dx} = \frac{y - xy/5 - Hy}{-x + xy/10 - Hx}
$$
 (2.14)

and vice-versa. Writing ODE  $(2.14)$  in differential form we have

<span id="page-5-3"></span>
$$
(y - xy/5 - Hy)dx + (x - xy/10 + Hx)dy = 0.
$$
 (2.15)

To separate the variables, divide ODE  $(2.15)$  through by xy to obtain the separated ODE

$$
\left(\frac{1-H}{x} - \frac{1}{5}\right)dx + \left(\frac{1+H}{y} - \frac{1}{10}\right)dy = 0.
$$



<span id="page-6-4"></span>Figure 4: Graph for  $(2.21)$ .

Integrating, we have the level curves

<span id="page-6-0"></span>
$$
(1 - H)\ln|x| - \frac{x}{5} + (1 + H)\ln|y| - \frac{y}{10} = C
$$
 (2.16)

where  $C$  is a constant. To find the level curve which passes through the point  $(8, 16)$  we set

$$
C = (1 - H) \ln |8| - \frac{8}{5} + (1 + H) \ln |16| - \frac{16}{10}
$$

and substitute this value for  $C$  back in  $(2.16)$  to get that

<span id="page-6-1"></span>
$$
(1 - H)\ln\frac{|x|}{8} + (1 + H)\ln\frac{|y|}{16} - \frac{1}{5}(x - 8) = \frac{1}{10}(y - 16)
$$
 (2.17)

as the equation of the level curve passing through the point (8, 16) for any value of  $H > 0$ . Rewriting equation  $(2.17)$  as

<span id="page-6-2"></span>
$$
H\left(\ln\frac{|y|}{16} - \ln\frac{|x|}{8}\right) - \frac{x}{5} - \frac{y}{10} + \frac{16}{5} + \ln\frac{|x|}{8} + \ln\frac{|y|}{16} = 0\tag{2.18}
$$

we see that a point  $(x, y)$  in the quadrant  $x > 0, y > 0$  satisfies equation  $(2.18)$  for all  $H > 0$ if and only if

<span id="page-6-3"></span>
$$
\ln \frac{y}{16} - \ln \frac{x}{8} = 0
$$
  
and 
$$
-\frac{x}{5} - \frac{y}{10} + \frac{16}{5} + \ln \frac{x}{8} + \ln \frac{y}{16} = 0.
$$
 (2.19)

Thus,  $y = 2x$  and from the first equation in  $(2.19)$  substituting this into the second equation we have that

<span id="page-7-1"></span> $-\frac{2}{7}$ 5  $x + \frac{16}{5}$ 5  $+ 2 \ln \frac{x}{g}$ 8  $= 0$  $e^{(x-8)/5} = \frac{x}{8}$ 8  $(2.20)$ 

or

The question now is this: does equation  $(2.20)$  have any solution for  $x > 0$  other than  $x = 8$ ? Using a graphical approach, put

<span id="page-7-0"></span>
$$
z = e^{(x-8)/5}
$$
 and  $z = \frac{x}{8}$  (2.21)

and plot these two curves in the  $zx$ -plane to see where they intersect. The graph in Figure [4](#page-6-4) shows that these two curves intersect in exactly two places:  $x = 8$  and  $x \approx 3$ .

Hence, there are exactly two points in the  $xy$ -plane that are common to all the orbits of the IVP  $(2.13)$  for all  $H > 0$ .

<span id="page-7-4"></span>Example 2.3 (Minimal Time of Descent). Here is an example where it is much more convenient to use a numerical solver rather than slog through the algebra of solution formulas.

A parachutist wants to jump out of a plane at 1200 ft and reach the ground going no more than 40 ft/sec and in minimal time (think James Bond landing behind enemy lines). (See Drucker  $[4]$ .) The parachutist's weight, including equipment, is 240 lbs. Air resistance has been found experimentally to be proportional to velocity with the proportionality constant  $k = 2$  during free fall and  $k = 10$  when the chute is open (assume that the chute opens instantaneously). Here are two questions to be answered:

- 1. What is the last possible moment that the chute can be deployed so that the parachutist lands at a speed no greater than 40 ft/sec?
- 2. What is the minimal time required for the parachutist to land at a speed no greater than than 40 ft/sec?

If m is the mass of the parachutist, including equipment, then  $mq = 240$ , where  $q = 32$ ft/sec<sup>2</sup>) is the gravitational constant. If  $y$  measures the height above the ground, then Newton's Second Law says that

<span id="page-7-2"></span>
$$
my'' = -mg - ky'
$$
 (2.22)

Putting  $v = y'$  and dividing through by m, ODE [\(2.22\)](#page-7-2) becomes

<span id="page-7-3"></span>
$$
v' + \frac{k}{m}v = -g.\tag{2.23}
$$

The solution of ODE [\(2.23\)](#page-7-3) with the initial condition  $v(0) = 0$  is

$$
v(t) = \frac{mg}{k}e^{-kt/m} - \frac{mg}{k}.
$$

So when the chutist jumps out of the plane his downward velocity increases until it hits the limiting velocity  $-mq/k$ . Hence, if the chute always remains closed (so  $k = 2$ ), then the chutist would hit the ground with velocity no greater than 120 ft/sec in magnitude. On the other hand, if the chutist jumped out of the plane with the chute open  $(k = 0)$ , then the chutist would hit the ground with velocity no more than 24 ft/sec. The solution formula for the IVP

<span id="page-8-0"></span>
$$
y'' = -g - \frac{kg}{240}y', \quad y(0) = 1200, \quad y'(0) = 0 \tag{2.24}
$$

is sufficiently complicated that it is difficult to answer the questions posed above just from that formula. So instead we shall use a numerical ODE solver. Toward that end let's first convert IVP [\(2.24\)](#page-8-0) into an equivalent normalized first-order system by setting  $x_1 = y$  and  $x_2 = y'$ , to obtain the system

<span id="page-8-2"></span><span id="page-8-1"></span>
$$
x'_1 = x_2
$$
  

$$
x'_2 = -g - \frac{kg}{240}x_2.
$$

Now comes the crucial step in this approach: to find the minimum time of descent in order for the chutist to land not faster than 40 ft/sec, proceed as follows: In the  $x_1x_2$  state space solve the IVP with the chute closed

$$
x'_1 = x_2, \t x_1(0) = 1200 \t (2.25)
$$

$$
x_2' = -32 - (4/15)x_2, \qquad x_2(0) = 0 \qquad (2.26)
$$

forward in time, and the IVP with the chute open

$$
x'_1 = x_2, \t x_1(0) = 0 \t (2.27)
$$

$$
x_2' = -32 - (4/3)x_2, \qquad x_2(0) = -40 \qquad (2.28)
$$

backward in time. IVP  $(2.26)$  describes the motion of the chutist from a height of 1200 ft with the chute closed. In IVP  $(2.28)$  the chutist starts with chute open at ground level and going -40ft/sec and is solved backwards in time. Plotting these two orbits in the state space  $0 \le x_1 \le 1200$ ,  $-120 \le x_2 \le 0$  yields the graph in Figure [5.](#page-9-0)

Zooming in near the point where the two curves in Figure [5](#page-9-0) intersect, we obtain Figure [6](#page-9-1) and see from this graph that the chutist must deploy his chute when  $x_1 \approx 88.7$ ft (and falling at a velocity of <sup>−</sup>116.<sup>1</sup> ft/sec) in order to land at -40 ft/sec. Deploying the chute *after*  $x_1 \approx 88.7$  ft will result in the chutist landing faster than 40 ft/sec. Deploying the chute *before*  $x_1 \approx 88.7$  feet would result in the chutist landing at slower than 40 ft/sec.

To find out when the chutist should pull the ripcord, solve the forward IVP [\(2.26\)](#page-8-1) and plot  $x_1$  versus t, zooming in on the screen 80  $\leq x_1 \leq 100$ , 12.75  $\leq t \leq 13$  to get Figure [7.](#page-10-0) From the graph in Figure [7](#page-10-0) we see that  $x_1 \approx 88.7$  when  $t \approx 12.88$  sec. Now the question is this: assuming the chute deploys instantaneously, how long is it before the chutist hits the ground? To find how long it takes for the chutist to hit the ground after his chute deploys solve the IVP [\(2.28\)](#page-8-2) backwards in time and plot  $x_1$  versus t for the solution to obtain the graph in Figure [8,](#page-10-1) after zooming in to the screen  $0 \le x_1 \le 100, -2.5 \le t \le 0$ .



<span id="page-9-0"></span>Figure 5: Solving IVP [\(2.26\)](#page-8-1) forward; IVP [\(2.28\)](#page-8-2) backward.



<span id="page-9-1"></span>Figure 6: Zoom of graph in Figure [5.](#page-9-0)

We see that  $x_1 \approx 88.7$  when  $t \approx 1.3$  sec. Therefore, the minimum time it takes the chutist to descend from 1200 ft in order to hit the ground at a speed of no more than 40 ft/s is approximately  $12.88 + 1.3 = 14.18$  sec.

With these figures we would not want to take the chutist's place. For one thing, chutes

<span id="page-10-0"></span>

<span id="page-10-1"></span>Figure 8: Zoom of solution of IVP [\(2.28\)](#page-8-2) backward.

don't open instantaneously, and for another thing the reaction time of the chutist to pull the ripcord is something on the order of <sup>1</sup>.<sup>3</sup> sec. Our guess is that the chutist would actually hit the ground at about 100 mi/hr if he follows this plan. So the safest thing to do would be to give up on this plan to reach the ground in minimum time.

#### 3 Autocatalators; An Example

In 1974 J. Arthur Campbell (a chemist known to students at Harvey Mudd College as "J. Arthur God"), Dick Popkin (a philosopher at Harvey Mudd College) and I (Courtney Coleman, a mathematician at Harvey Mudd College and the author of this segment) tackled the question "What is Truth?". The setting was a seminar at the Claremont Graduate School (now called Claremont Graduate University). Art Campbell opened the seminar and spoke about chemical kinetics and how chemical reactions evolve. He pointed out that most chemists believed that all chemical reactions proceeded steadily toward end products (a chemical "truth"). Then he combined liquids in a flask, stirred them up, set the flask on a table and sat down. From that point on, no one paid any attention to what Campbell, Popkin or I had to say. All eyes were on the events taking place in the flask, marked as they were by oscillating changes in color back and forth between blue and clear states, but eventually coming to an end. These reactions seemed to be going backwards as well as forwards! So what is going on here?

A chemical reaction like that described above was seen in 1951 by the Russian chemist Boris Belousov (1894–1970). He observed a specific chemical reaction that behaved as if it were promoting its own production. He reported on what he observed, but no one believed him and his work was ignored. In disgust, he abandoned his research and it was only years later that its importance was recognized. The reaction is now known as the B-Z Reaction, named after Belousov and A. N. Zhatbotinsky, another early pioneer in this area of chemical research. Belousov had a turbulent life, starting out as a revolutionary in the tsarist days. After the Bolshevik revolution of 1917 he joined the army and rose to the rank of Brigade Commander. Eventually he got out of the army and began a career as a research chemist. A decade after his death his work was recognized with the highest civilian award of the Soviet era.

It was only many years after the "Truth" seminar that the book by Gray and Scott  $\lceil 5 \rceil$ appeared. When I later discovered this book I realized that what had been going on in the flask at the seminar was something called autocatalysis. Autocatalysis is a process by which a substance promotes (i.e., catalyses) its own production, but in the process may generate other chemical species which in turn regenerate the original substance. This can sometimes be observed as oscillating colors. Here are some terms that appear in articles where this phenomenon is discussed:

Catalator (or Catalyst): an agent that brings about or facilitates a change. Catalysis: the action of a catalator that increases the rate of change without the catalator itself being consumed. *Catalyse:* to accelerate or promote a process or reaction by catalysis. Autocatalator: an agent that promotes its own production. Autocatalysis: the catalysis of a reaction by one of its own products. Autocatalyse: to accelerate or promote a process or reaction by autocatalysis.

These definitions are generic, but in this article they specifically refer to chemical reactions and the mathematical equations for the rates at which the reactions proceed. When modeling physical phenomena with mathematical equations, numerical solutions of those equations may exhibit artifacts not actually present in the phenomena. However, in the autocatalator example described below the unusual numerical solution does indeed correspond to the actual physical behavior.

Example 3.1 (An Autocatalator). A species in a chemical reaction is a catalator if it promotes the reaction. The species is an autocatalator if it promotes its own production in the reaction. Here is an example of a reaction with an autocatalytic step.

<span id="page-12-5"></span>

The process stops after the supply of the precursor species R runs out. This example is discussed in some detail in Differential Equations: A Modeling Perspective [\[1\]](#page-16-3), pg. 445; in Borrelli et al. [\[3\]](#page-16-6), pg. 247; and in Borrelli and Coleman [\[2\]](#page-16-2).

A basic law of chemistry provides the transition from the four reaction steps to four rate equations.

Chemical Law of Mass Action In each step of a chemical reaction the rate of decrease of the concentration of each reactant species is proportional to the arithmetic product of the concentrations of all the reactant species. Similarly, the rate of increase of the concentration of each product chemical is proportional to the arithmetic product of the concentrations of all the reactants.

Similarly, the rate of increase of the concentration of each product chemical is proportional to the product of the concentrations of all the reactants.

The Mass Action Law provides the rate equations

<span id="page-12-6"></span><span id="page-12-0"></span>
$$
dw/dt = -aw \tag{3.5}
$$

<span id="page-12-3"></span><span id="page-12-1"></span>
$$
dx/dt = aw - bx - cxy^2 \tag{3.6}
$$

$$
dy/dt = bw - ky + cxy2
$$
 (3.7)

<span id="page-12-4"></span><span id="page-12-2"></span>
$$
dz/dt = ky,\t\t(3.8)
$$

where w, x, y, z denote the scaled concentrations of the respective chemical species R,A,B,C and  $a, b, c, k$  are positive rate constants. The Mass Action Law explains why the sum  $A + 2B$  in the autocatalytic step [\(3.3\)](#page-12-0) becomes  $xy^2$  in the rate equations [\(3.6\)](#page-12-1) and [\(3.7\)](#page-12-2). Note that the total concentration is constant over time since  $d(w + x + y + z)/dt = 0$ .

The rate equation for  $w(t)$  is linear and its solution is  $w(t) = w(0)e^{-at}$ , where  $w(0)$ is the initial value of w. So  $w(t)$  decays exponentially as t increases. The next two rate equations are nonlinear because of the term  $xy^2$ . Solutions of these rate equations cannot be expressed in terms of the familiar functions of calculus. Instead we turn to the numerical differential equation solver ODE Architect to generate tables of approximate solution values, given the specific values used by Gray and Scott  $[5]$ :

<span id="page-12-7"></span>
$$
w(0) = 500
$$
  
\n
$$
x(0) = y(0) = z(0) = 0
$$
  
\n
$$
a = 0.002 \quad b = 0.08 \quad c = 1 \quad \text{and} \quad k = 1.
$$
\n(3.9)



<span id="page-13-0"></span>Figure 9: Decline in the concentration of the precursor species

These approximate solution values can be used to plot  $w(t)$ ,  $x(t)$ ,  $y(t)$  and  $z(t)$  against t.

Figure  $\theta$  shows the decline of the precursor species R (denoted by w) as the process goes on. Figure [10](#page-14-0) shows small oscillations in the intermediates A and B (denoted by  $x$ and  $\gamma$  respectively). These correspond, respectively, to the blue and the clear states noted in the Campbell experiment mentioned earlier. Figure [11](#page-15-0) shows the increase over time of the end-product C (denoted by z). The oscillations in the intermediates do not seem to have much effect on the end-product (but see the small amplitude wiggles in Figure [11\)](#page-15-0). Note the different vertical scales in the figures.

Gray and Scott, [\[5\]](#page-16-5), also list specific chemical mixtures that display oscillating color changes. Perhaps it was one of these chemical mixtures that was observed in the "Truth" seminar in 1974.

#### 3.0.1 Comments

Attempts to use a mathematical model to represent an observed physical phenomenon should address the following questions.

- 1. Are the physical principles that underlie the phenomenon accurately modeled by mathematical equations?
- 2. Do the solutions of the mathematical equations accurately portray the behavior of the physical phenomenon?



<span id="page-14-0"></span>Figure 10: Oscillations in the concentration of the intermediates,  $A$  (top) and  $B$  (bottom).

3. Is the mathematical model robust? In particular, do the actual physical effects of small changes in the conditions of the phenomenon match up well with the effects of the corresponding small changes in the model equations on the solutions of those equations?

Here are some specific questions about the autocatalator model.

- 4. Are the oscillatory solutions of the mathematical equations  $(3.5)-(3.8)$  $(3.5)-(3.8)$  $(3.5)-(3.8)$  in this model real or are they artifacts of the numerical methods used to find approximate solutions of the equations?
- 5. For the chemical system  $(3.1)$ – $(3.4)$  modeled by differential equations  $(3.5)$ – $(3.8)$ , is the model robust?
- 6. In actual chemistry experiments the oscillating changes die out over time and equilibrium is approached. The graphs in Figures [10](#page-14-0) and [11](#page-15-0) suggest the same behavior in solutions of equations  $(3.5)-(3.8)$  $(3.5)-(3.8)$  $(3.5)-(3.8)$ .
- 7. These issues are addressed in detail in reference Gray and Scott  $[5]$ . The conclusion is that the model seems to be robust and that oscillatory solutions of the model equations accurately correspond to the observed oscillations in the colors of the chemical compounds.
- 8. In numerical simulations large initial values of the precursor seem to suppress the



<span id="page-15-0"></span>Figure 11: The oscillations in  $x(t)$  and  $y(t)$  have small effect on  $z(t)$ .

oscillations in the intermediates? Is this true in the chemical experiments? Scott [\[7\]](#page-16-7) discusses many examples of chemical oscillations.

### 4 Suggested Exercises

- 1. Would it take a ball longer to rise or to fall on the moon? On Mars?
- 2. Prove that a straight line cuts the graph of  $y = e^x$  twice, once, or not at all.
- 3. See if you can find more accurate values for the coordinates of the second fixedpoint identified in Example [2.2.](#page-4-3) [You might try successive approximation to solve equation  $(2.20)$ ].
- 4. In Example [2.2,](#page-4-3) the system of equations [\(2.11\)](#page-4-4) models predator-prey interactions with proportional harvesting. The parameters  $a, b, c, d$  and  $H$  are positive constants. Let  $(x_0, y_0)$  be a point inside the positive quadrant of the xy-plane. Consider all the orbits of the predator-prey model above for  $H > 0$  that pass through the point  $(x_0, y_0)$ . Show that exactly one of the following statements is true:
	- (a) If  $dx_0 + by_0 = c + a$ , then  $(x_0, y_0)$  is the only point in the xy-plane which is common to all the orbits.
	- (b) If  $dx_0 + by_0 > c + a$ , then there is exactly one more point  $(x_1, y_1)$  in the xy-plane common to all the orbits, and  $x_1 < x_0$ .
	- (c) If  $dx_0 + by_0 < c + a$ , then there is exactly one more point  $(x_1, y_1)$  in the xy-plane common to all the orbits, and  $x_1 > x_0$ .

Choose various specific positive values for a, b, c, d,  $x_0$  and  $y_0$  and use a numerical solver/grapher to illustrate the validity of statements (b) and (c). Which statement applies to the predator-prey problem in Example [2.2?](#page-4-3) It is a bit trickier to use a numerical solver to illustrate statement (a). Why?

- 5. Can you modify the landing speed, the initial height of the chutist and/or the viscous drag coefficients to obtain more reasonable results for Example [2.3?](#page-7-4)
- 6. If the parachutist in Example [2.3](#page-7-4) were to start at an elevation of 1200 feet above the surface of Mars, could he in minimal time reach the surface of Mars traveling no faster than 40 ft/sec?
- 7. Using the autocatalator data given in  $(3.9)$  but replacing  $R(0)$  by  $R(0) = 1000, 750, 250,$ and finally  $R(0) = 100$ , describe what happens as the value of  $R(0)$  changes.
- 8. Can you turn off the oscillations by changing the value of <sup>a</sup> from <sup>0</sup>.<sup>002</sup> to <sup>0</sup>.02? <sup>0</sup>.2? 0.0002? Leave all other data as listed in  $(3.9)$ .

### References

- <span id="page-16-3"></span>[1] Robert L. Borrelli and Courtney Coleman. Differential Equations: A Modeling Perspective. J. Wiley and Sons, second edition, 2004. Included with the book is a CD-ROM with the numerical ODE solver, ODE Architect.
- <span id="page-16-2"></span>[2] Robert L. Borrelli and Courtney Coleman. Modelling and visualization with ODE Architect: An example set, 1999. URL [http://www.math.hmc.edu/resources/](http://www.math.hmc.edu/resources/odes/odearchitect/examples/) [odes/odearchitect/examples/](http://www.math.hmc.edu/resources/odes/odearchitect/examples/).
- <span id="page-16-6"></span>[3] Robert L. Borrelli, Courtney Coleman, and William E. Boyce. Differential Equations Laboratory Workbook: A Collection of Experiments, Explorations, and Modeling Projects for the Computer. John Wiley & Sons, Inc., New York, NY, USA, 1992. ISBN 0471551422.
- <span id="page-16-4"></span>[4] Jack Drucker. The computer corner of the CMJ. The College Mathematics Journal, 26 (23), May 1995.
- <span id="page-16-5"></span>[5] Peter Gray and Stephen K. Scott. *Chemical Oscillations and Instabilities*. Clarendon Press, Oxford, 1990.
- <span id="page-16-1"></span>[6] John H. Hubbard. The forced damped pendulum: Chaos, complication, and control. CODEE Newsletter, pages 3-11, Spring 1995. URL [http://ccdl.libraries.](http://ccdl.libraries.claremont.edu/u?/cla,127) [claremont.edu/u?/cla,127](http://ccdl.libraries.claremont.edu/u?/cla,127).
- <span id="page-16-7"></span>[7] Stephen K. Scott. Chemical Chaos. Clarendon Press, Oxford, 1994.
- <span id="page-16-0"></span>[8] Larry Shampine. Numerical Solution of Ordinary Differential Equations. Chapman and Hall/CRC, New York, March 1994.
- <span id="page-17-1"></span>[9] Lawrence Shampine. The savvy solver. CODEE Newsletter, pages 10–12, Fall 1992. URL <http://ccdl.libraries.claremont.edu/u?/cla,12>.
- <span id="page-17-2"></span>[10] Lawrence Shampine. The savvy solver II. CODEE Newsletter, pages 12–14, Winter 1993. URL <http://ccdl.libraries.claremont.edu/u?/cla,180>.
- <span id="page-17-3"></span>[11] Lawrence Shampine. The savvy solver III. CODEE Newsletter, pages 11–14, Spring 1993. URL <http://ccdl.libraries.claremont.edu/u?/cla,56>.
- <span id="page-17-4"></span>[12] Lawrence Shampine. The savvy solver IV. CODEE Newsletter, pages 5–7, Spring 1994. URL <http://ccdl.libraries.claremont.edu/u?/cla,25>.
- <span id="page-17-0"></span>[13] Ian Stewart. Warning: Handle with care! Nature, 355(6355):16–17, January 1992.