SIMIODE
LSD Modeling and Arithmetic Performance
Modeling Falling Column of Water
Yeast Modeling

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SIMIODE, Cornwall NY USA

Outline of Talk
SIMIODE Enables
Teaching Differential Equations with Modeling

▶ Overview of SIMIODE

▶ Modeling Scenarios - navigation, Resource Guide, Search

▶ Modeling Scenario on LSD and Arithmetic Performance

▶ Modeling Falling Column of Water

▶ Gause Yeast Modeling in the Soviet Union

▶ A word from our sponsors
  ▶ Moving to QUBES Hub at https://qubeshub.org/.
  ▶ SCUDEM and feature past bio problems and student videos.

All materials are available at www.simiode.org.

https://www.simiode.org/register

Registration is FREE.
Resources are Open Education Resources (OER).
All are downloadable and fully adaptable.

SIMIODE is funded by the National Science Foundation
Division of Undergraduate Education.

- ▶ StarterKit – SIMIODE Resource Guide – Sample Syllabus
- ▶ **Modeling Scenarios** and Technique Narratives
- ▶ Potential Modeling Scenarios – Activities Using Data
- ▶ Refereed publication of your materials
- ▶ Listing FREE online texts
- ▶ Winter 2020 SIMIODE online text
- ▶ SIMIODE EXPO - Online Conference 12-13 February 2021
- ▶ SCUDEM V 2020 - Registration open now
- ▶ SIMIODE Challenge Using Differential Equations Modeling
  - ▶ Challenge Period 23 Oct - 14 Nov 2020 - produce video
  - ▶ Three member student teams work on 1 of 3 models
  - ▶ Teams from one school or SIMIODE creates teams from individual student registrations from around the world
  - ▶ Students from Lagos NIGERIA, Prague CZECH REPUBLIC, Missoula MT USA, with Coach from Kyoto JAPAN
  - ▶ Opportunity to Coach local team or international team
  - ▶ We need Judges - watch three 10 minute videos

STUDENT VERSION

Drone Heading Home

Richard Spindler
Department of Mathematics
SUNY Plattsburgh
Plattsburgh NY USA

TEACHER VERSION

EBOLA OUTBREAK IN WEST AFRICA

Lisa Driskell
Computer Science, Mathematics, and Statistics
Colorado Mesa University
Grand Junction CO 81501 USA
ldriskel@coloradomesa.edu

TEACHER VERSION

Employee Attrition

Lyle Smith III
Mathematical & Physical Sciences
Bryan College
Dayton TN 37321 USA

TEACHER VERSION

MODELING THE STEEPING OF
SOUTHERN SWEET ICED TEA

Troy Henderson
Department of Mathematics
University of Mobile
Mobile AL 36613 USA

STUDENT VERSION

Simulating the Spread of the Common Cold

Richard Corban Harwood
Department of Mathematics
George Fox University
Newberg OR USA

TEACHER VERSION

MODELING BUBBLES OF BEER

Michael A. Karls
Department of Mathematical Sciences
Ball State University
Muncie, IN 47306 USA
mkarls@bsu.edu

TEACHER VERSION

At what age do people get married?

Tracy Weyand
Department of Mathematics
Rose-Hulman Institute of Technology
Terre Haute IN 47803 USA
weyand@rose-hulman.edu

TEACHER VERSION

M&M Attrition Warfare

Lukasz Grabarek
Department of Mathematics
Matanuska-Susitna College
University of Alaska Anchorage
8295 E College Dr. Palmer AK 99645 USA

TEACHER VERSION

Heat Diffusion

Kimberly Spayd and James Puckett
Department of Mathematics and Department of Physics
Gettysburg College
Gettysburg PA 17325 USA

TEACHER VERSION

MODELING A NONLETHAL INFLUENZA EPIDEMIC

Sheila Miller
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New York City College of Technology
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Modeling LSD in the Blood Stream and Tissues

	Time (hr)	0.0833	0.25	0.5	1.0	2.0	4.0	8.0
Subject 1	Plasma Conc (ng/ml)	11.1	7.4	6.3	6.9	5.	3.1	0.8
	Perform Score (%)	73	60	35	50	48	73	97
Subject 2	Plasma Conc (ng/ml)	10.6	7.6	7.	4.8	2.8	2.5	2.
	Perform Score (%)	72	55	74	81	79	89	106
Subject 3	Plasma Conc (ng/ml)	8.7	6.7	5.9	4.3	4.4	—	0.3
	Perform Score (%)	60	23	6	0	27	69	81
Subject 4	Plasma Conc (ng/ml)	10.9	8.2	7.9	6.6	5.3	3.8	1.2
	Perform Score (%)	60	20	3	5	3	20	62
Subject 5	Plasma Conc (ng/ml)	6.4	6.3	5.1	4.3	3.4	1.9	0.7
	Perform Score (%)	78	65	27	30	35	43	51

Summary of data collected on 5 male volunteers who were given LSD and then tested on simple addition questions.

Source: Metzler, C. M. 1969. A Mathematical Model for the Pharmacokinetics of LSD Effect. *Clinical Pharmacology and Therapeutics*. 10(5): 737-740.

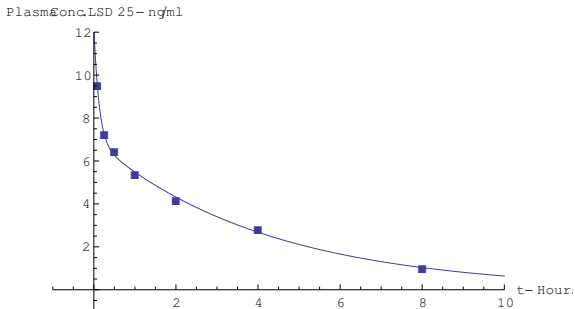Two compartment model for LSD flow between plasma and tissue compartments in the human body.
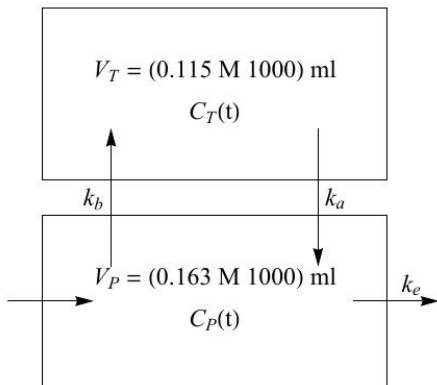
$$V_P C_P'(t) = k_a V_T C_T(t) - k_b V_P C_P(t) - k_e V_P C_P(t)$$
$$V_T C_T'(t) = k_b V_P C_P(t) - k_a V_T C_T(t).$$

$$SSE(k_a, k_b, k_e) = \sum_{i=1}^{7}(C_P(t_i) - O_i)^2 \qquad (1)$$

Minimizing $SSE(k_a, k_b, k_e)$ we obtain the parameters
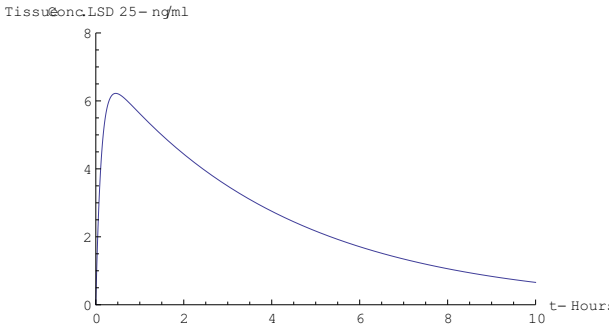$k_a = 4.63679$, $k_b = 3.18659$, and $k_e = 0.41128$.

Plasma Conc.LSD 25 − ng/ml

t − Hours

Plot of the observed values of the average concentration
of LSD (ng/ml) (squares)in plasma and the model.

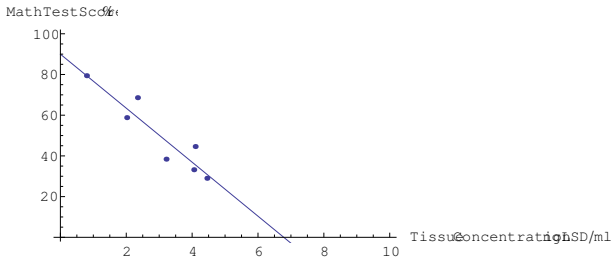$$C_P(t) = 0.128905 \left(41.2194 e^{-7.99617t} + 53.9669 e^{-0.238492t}\right).$$

$$C_T(t) = 0.128905 \left(55.419 e^{-0.238492t} - 55.419 e^{-7.99617t} \right).$$

Plot of the model of tissue concentration of LSD in ng/ml.

This means with a model we can watch the concentration of LSD in the body tissue over time from just observing the concentration of LSD in the plasma (or blood) from regular draws.

Plot of Performance Score (%) (*PS*) on the simple arithmetic problems vs. the model prediction of the concentration of LSD in ng/ml in the tissue compartment (*CT*).

This means for every ng/ml increase in LSD in the tissue compartment the score drops a little over 9 points.

Modeling Falling Column of Water

We collect data on a falling column of water and model the height using first principles from physics with a differential equation.
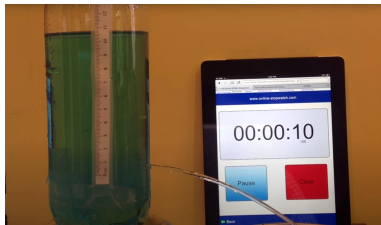
1. Video, data, qualitative behavior, empirical model

2. First principles analytic model, Torricelli's Law

3. Differential equation, estimate parameters, validate model

4. Discussions

Source:
1-015-S-Torricelli **https://www.simiode.org/resources/488**
1-015-T-Torricelli **https://www.simiode.org/resources/463**

We use data taken from video at SIMIODE YouTube Channel


https://www.youtube.com/watch?v=NBr4DOj4OTE .

Cylindrical column (radius $= 4.17$ cm) of water empties through a hole (diameter $= 11/16" = 0.218281$ cm) in bottom of column. Exit hole at bottom of column - height is 0 cm.

We seek to model $h(t)$, the height of the column of water.

Stop and start to collect data.
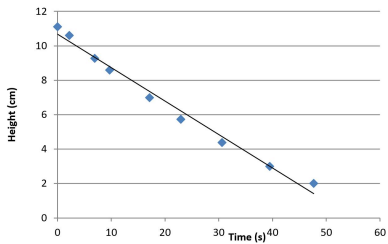
Here is data we collected.

Time (s)	Height (cm)
0.0	11.1
2.187	10.6
6.933	9.3
9.717	8.6
17.102	7.0
22.968	5.75
30.603	4.4
39.503	3.0
47.663	2.0
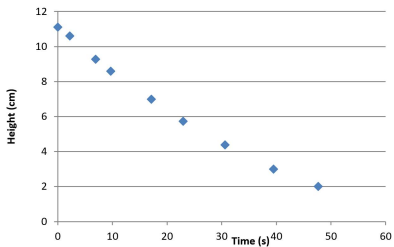
Linear Fit?

Time (s)	Height (cm)
0.0	11.1
2.187	10.6
6.933	9.3
9.717	8.6
17.102	7.0
22.968	5.75
30.603	4.4
39.503	3.0
47.663	2.0

Exponential Decay Fit?

Time (s)	Height (cm)
0.0	11.1
2.187	10.6
6.933	9.3
9.717	8.6
17.102	7.0
22.968	5.75
30.603	4.4
39.503	3.0
47.663	2.0
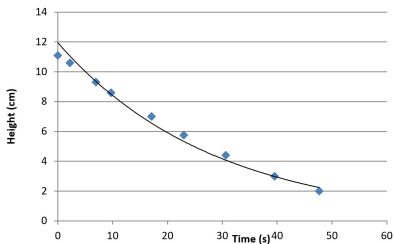
All are empirical fits with no understanding.

They just fit a function to data.

And neither line nor exponential are good.

What happens to height $h(t)$?

How fast is column of water falling? Early and later?

Time (s)	Height (cm)
0.0	11.1
2.187	10.6
6.933	9.3
9.717	8.6
17.102	7.0
22.968	5.75
30.603	4.4
39.503	3.0
47.663	2.0

Check out the average rate of falling of the height of the column of water in several intervals, say, $[0, 2.187]$,

$$\frac{10.6 - 11.1}{2.187 - 0} = -0.2286\,,$$

or in the interval $[39.503, 47.663]$,

$$\frac{2.0 - 3.0}{47.663 - 39.503} = -0.122549\,.$$

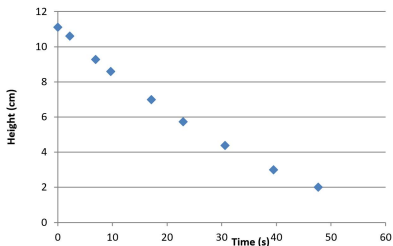What do you see? What can you say about $h'(t)$?

Let's find a model from some first principles.

This would be an analytic model.

NOT just fit a function to data.

NOT just "it looks like it falls faster or slower."

Time (s)	Height (cm)
0.0	11.1
2.187	10.6
6.933	9.3
9.717	8.6
17.102	7.0
22.968	5.75
30.603	4.4
39.503	3.0
47.663	2.0

Enter Evangelista Torricelli 1608–1647, an Italian physicist and mathematician, and a student of Galileo. Best known for his invention of the barometer and his wicked mustache!

Torricelli's Law to the rescue!

$$\frac{dh(t)}{dt} = -b\sqrt{g \cdot h(t)}, \quad h(0) = h_0 \quad b > 0.$$

Say it out loud in sentence form.

Explain to yourself what it means.

Does Torricelli's Law agree with observations?

For large $h(t)$ the column of water falls faster or slower ....

For small $h(t)$ the column of water falls faster or slower ....

We derive Torricelli's Law from Conservation of Energy Principle.

Now by The Law Conservation of Energy - Initial Total Energy equals Final Total Energy.

$$TE_i = \frac{1}{2}mv_i^2 + mgh = \frac{1}{2}mv_f^2 = TE_f \,,$$

Divide both sides by m and multiply by 2 - to solve for v_f:

$$v_f = \sqrt{2gh + v_i^2} \,.$$

Since $v_i = 0$ we have one classical form of Torricelli's Law

$$v_f = \sqrt{2gh} \,,$$

where v_f is the speed of the water as it leaves the exit hole.

So we have an analytic model (differential equation!) for $h(t)$.

$$\frac{dh(t)}{dt} = -b\sqrt{g \cdot h(t)}, \quad h(0) = h_0 \,.$$

We solve this differential equation for $h(t)$ to realize a model.

What strategy/technique can we employ? What technology?

We use this solution and our data to estimate parameter b and validate our model by comparing model predictions to data.

$$\frac{dh(t)}{dt} = -b\sqrt{g \cdot h(t)} = -b\sqrt{g} \cdot (h(t))^{1/2}.$$

Separate the variables

$$(h(t))^{-1/2} \cdot \frac{dh(t)}{dt} = -b\sqrt{g}.$$

OR

$$(h(t))^{-1/2} \cdot dh = -b\sqrt{g} \cdot dt.$$

Integrate both sides. (What is C?)

$$\int (h(t))^{-1/2} \cdot \frac{dh(t)}{dt} \, dt = \int -b\sqrt{g} \, dt + C,$$

$$2(h(t))^{1/2} = -b\sqrt{g} \cdot t + C.$$

Now to find C using Initial Conditions:

$$2(h(t))^{1/2} = -b\sqrt{g} \cdot t + C.$$

$$2(h(0))^{1/2} = -b\sqrt{g} \cdot 0 + C = C.$$

Thus we have

$$2(h(t))^{1/2} = -b\sqrt{g} \cdot t + 2(h(0))^{1/2}.$$

Divide both sides by 2 and then square both sides yields:

$$h(t) = \left(-\frac{b\sqrt{g}}{2} \cdot t + (h(0))^{1/2}\right)^2. \qquad (2)$$

This is model for height of the column of water, $h(t)$, at time t.

What do we know and what do we need to estimate b in (2)?

$h(0) = 11.1$ cm and $g = 980$ cm/s^2

Thus from $h(0) = 11.1$ cm and $g = 980$ cm/s^2

$$h(t) = \left(-\frac{b\sqrt{g}}{2} \cdot t + (h(0))^{1/2}\right)^2$$

becomes

$$h(t) = \left(-\frac{b\sqrt{980}}{2} \cdot t + (11.1)^{1/2}\right)^2,$$

and expanded in decimals we have

$$h(t) = \left(-15.6525 \cdot b \cdot t + 3.33166\right)^2. \tag{3}$$

We have arrived at our model and now we seek to determine b and validate our model.

We turn to our Excel spreadsheet and seek to determine the parameter b which minimizes the sum of the squared errors between our data (h_i) and our model $(h(t_i))$ over our data points.

$$SSE(b) = \sum_{i=1}^{9} (h_i - h(t_i))^2 .$$

Minimize as a function of the parameter b:

$$SSE(b) = \sum_{i=1}^{9} (h_i - h(t_i))^2 .$$

where

- t_i is the ith time observation,
- h_i is the observed height at time t_i,
- $h(t_i)$ is our model's prediction of the height at time t_i, and
- $n = 9$ is the number of data points we have.

Model Analysis in Excel Using Solver

Data collected Friday, 5 August 2016 by Brian Winkel

SOURCE for Data
https://www.youtube.com/watch?v=NBr4DOj4OTE
Radius of hole 11/64" = 0.218281 cm and radius of cylinder 4.17 cm

Model h'(t) = -b Sqrt(g h(t))

Model h(t) = (-b Sqrt(g)/2 + h(0)^(1/2))^2

|				b=	0.002
	Zeroed	Actual	Model	SSE	
Time (s)	Time	Height (cm)			
8.679	0	11.1	11.09995836	1.73426E-09	
10.866	2.187	10.6	10.64844791	0.0023472	
15.612	6.933	9.3	9.700872913	0.160699092	
18.396	9.717	8.6	9.165570453	0.319869938	
25.781	17.102	7	7.819192408	0.671076202	
31.647	22.968	5.75	6.825923093	1.157610501	
39.282	30.603	4.4	5.634134022	1.523086785	
48.182	39.503	3	4.389102871	1.929606788	
56.342	47.663	2	3.384016994	1.915503039	
			Total SEE	7.679799546	
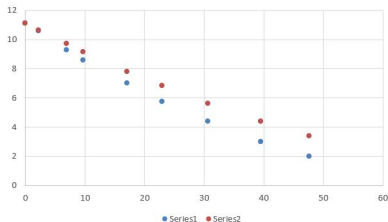
We can use Excel's Solver to minimize the TOTAL SEE or SSE
which is currently 7.679799546 with parameter $b = 0.002$ by asking
Solver to minimize SEE or SSE as a function of $b = 0.002$ cell.

Parameter Estimation with Excel Solver - Results

Model h'(t) = -b Sqrt(g h(t))

Model h(t) = (-b Sqrt(g)/2 + h(0)^(1/2))^2

				b=	0.002581
	Zeroed	**Actual**	**Model**	**SSE**	
Time (s)	**Time**	**Height (cm)**			
8.679	0	11.1	11.09995836	1.73426E-09	
10.866	2.187	10.6	10.51908638	0.006547014	
15.612	6.933	9.3	9.312232219	0.000149627	
18.396	9.717	8.6	8.638501405	0.001482358	
25.781	17.102	7	6.973871293	0.000682709	
31.647	22.968	5.75	5.778477118	0.000810946	
39.282	30.603	4.4	4.390799244	8.46539E-05	
48.182	39.503	3	3.013347567	0.000178158	
56.342	47.663	2	1.977592125	0.000502113	
			Total SEE	0.010437581	

Model (Red) and Data (Blue)
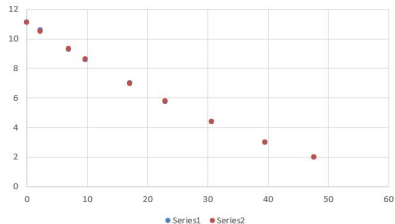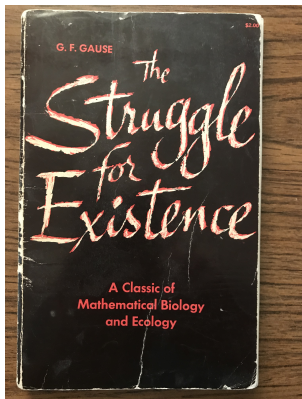
We study models of yeast growth by G. F. Gause on the way to improving vodka production in the Soviet Union. Species separately and together, competitive model and parameter estimation to see niche overlap.

Gause modeled each species separately to discover their r and K

$$
\begin{aligned}
\frac{dN_1}{dt} &= r_1 N_1 \frac{K_1 - N_1}{K_1}, \\
\frac{dN_2}{dt} &= r_2 N_2 \frac{K_2 - N_2}{K_2}.
\end{aligned}
$$

He then used these values of r and K to estimate parameters α and β which he called "coefficients for the struggle for existence".

$$\frac{dN_1}{dt} = r_1 N_1 \frac{K_1 - \alpha N_2 - N_1}{K_1}$$

$$\frac{dN_2}{dt} = r_2 N_2 \frac{K_2 - \beta N_1 - N_2}{K_2}$$

Knowing α and β helped determine part of the interaction between these two species of yeast so he would know what would happen in mixed populations of yeast.

All this work was done in the 1930's BY HAND, e.g., using rulers on hand plots to approximate derivatives!

Age in hours	Saccharomyces Volume of yeast	Mixed Population Volume of yeast	Schizosaccharomyces Volume of yeast	Mixed Population Volume of yeast
6	0.37	0.375	-	0.291
16	8.87	3.99	1.00	0.98
24	10.66	4.69	-	1.47
29	12.50	6.15	1.70	1.46
40	13.27	-	-	-
48	12.87	7.27	2.73	1.71
53	12.70	8.30	-	1.84
72	-	-	4.87	-
93	-	-	5.67	-
117	-	-	5.80	-
141	-	-	5.83	-
7.5	1.63	0.923	-	0.371
15.0	6.20	3.082	1.27	0.630
24.0	10.97	5.780	-	1.220
31.5	12.60	9.910	2.33	1.112
33.0	12.90	9.470	-	1.225
44.0	12.77	10.570	-	1.102
51.5	12.90	9.883	4.56	0.961

We see the growth of the yeast volume and the number of cells in pure cultures of *Saccharomyces cerevisiae* (column 1), *Schizosaccaromyces kefir* (column 3) and in the mixed population of these species (column 2 and 4 respectively).

Here is an activity for students:

Estimate the respective parameter sets, r_1 and K_1 and then r_2 and K_2, for Gause's two separate populations in the two separate logistic equations using the appropriate data in the table.

We share Gause's estimates for r and K for each of the two population models in his published works and we include these values below for you to compare your work with his.

	Your Analysis		Gause's Analysis	
Species	r	K	r	K
Saccharomyces			0.21827	13.0
Schizosaccharomyces			0.06069	5.8

Using Mathematica we compute the sum of the square errors (SSE) between a model and our data for thousands of values of α and β over a grid to see where the minimum SSE lies.
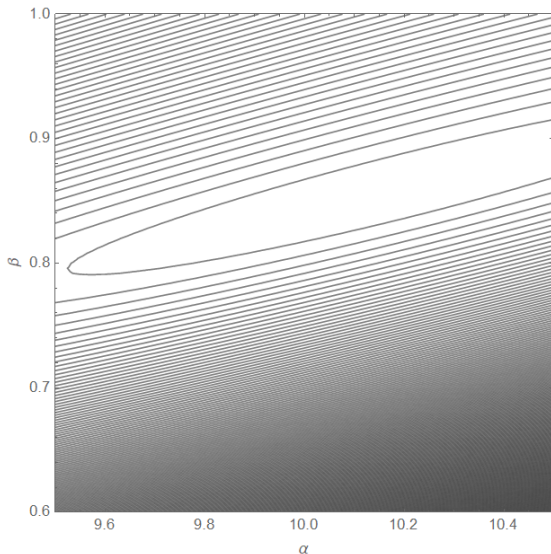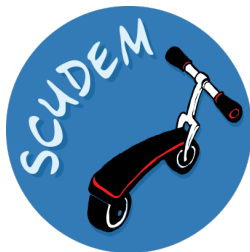
We render a plot of the full competitive model with best fitting parameters over the data .

$$\frac{dN_1}{dt} = r_1 N_1 \frac{K_1 - \alpha N_2 - N_1}{K_1}$$

$$\frac{dN_2}{dt} = r_2 N_2 \frac{K_2 - \beta N_1 - N_2}{K_2}$$

Model and Data Plot
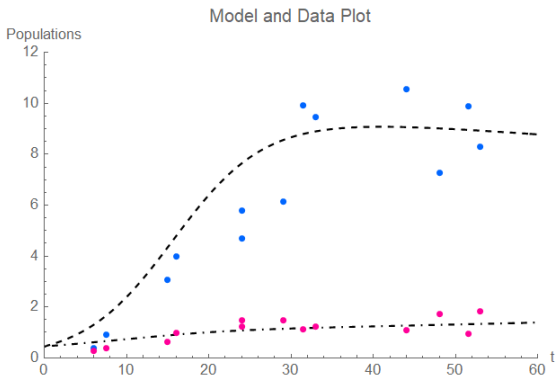
A word from one of our sponsors . . . .

https://www.simiode.org/scudem

OR just search "SCUDEM" in Google.

Fall 2020 with Challenge Saturday due date 14 November 2020.

Features of SCUDEM V 2020 (**www.simiode.org/scudem**)

- ▶ teams of three high school, home school, individuals, or undergraduate students - undergraduate level or lower

- ▶ teams from same institution or assembled by SIMIODE from students around the world

- ▶ mentor/coach faculty engage with teams and fellow mentors/coaches

- ▶ mentoring period 1 September 2020 through 23 October 2020

- ▶ three problems from physics/engineering, chemistry/life sciences, and social sciences/humanities released on 23 October 2020

- ▶ students prepare 10 minute video presentation and upload to YouTube by Challenge Saturday, 14 November 2020

- ▶ faculty from around the world judge and give feedback

- ▶ Outstanding, Meritorious, and Successful awards

- ▶ SIMIODE posts ALL student team submissions and essay by problem poser on student submissions.

Discussions and Questions
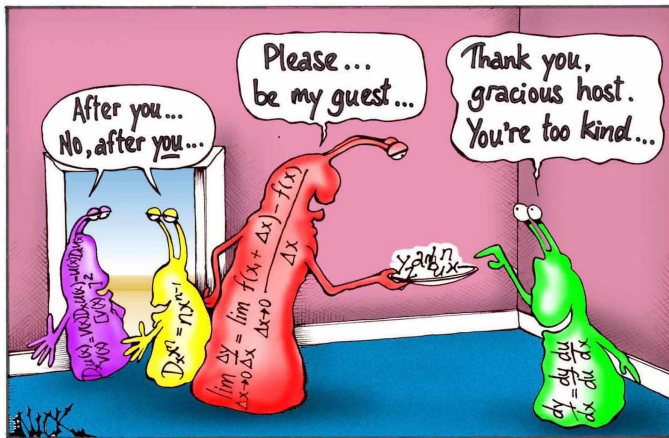
Deferential equations.

Join us at SIMIODE and
take the lead for modeling with differential equations.
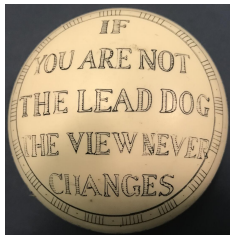
Visit us at **SIMIODE** and register.

All is FREE at SIMIODE!