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SIMIODE

A SYSTEMIC INITIATIVE FOR MODELING INVESTIGATIONS & OPPORTUNITIES WITH DIFFERENTIAL EQUATIONS

WELCOME! Thank you for joining us.

SCUDEM 2017 – Faculty Development Workshop
Mount Saint Mary College, Newburgh NY USA

SCUDEM

Student Competition Using Differential Equation Modeling

Brian Winkel, Director SIMIODE
Emeritus Prof MathSci, US Military Academy, West Point NY USA

Themes:

* Browsing and finding modeling activities ideas.
* SIMIODE as source.
* Modeling LSD
* m&m death and immigration modeling – collect data, build model
* Torricelli's Law for falling column of water –video to collect data and model

Other examples: Tuned Mass Dampers and Falling Shuttlecock

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Browsing Your Way to Better Teaching

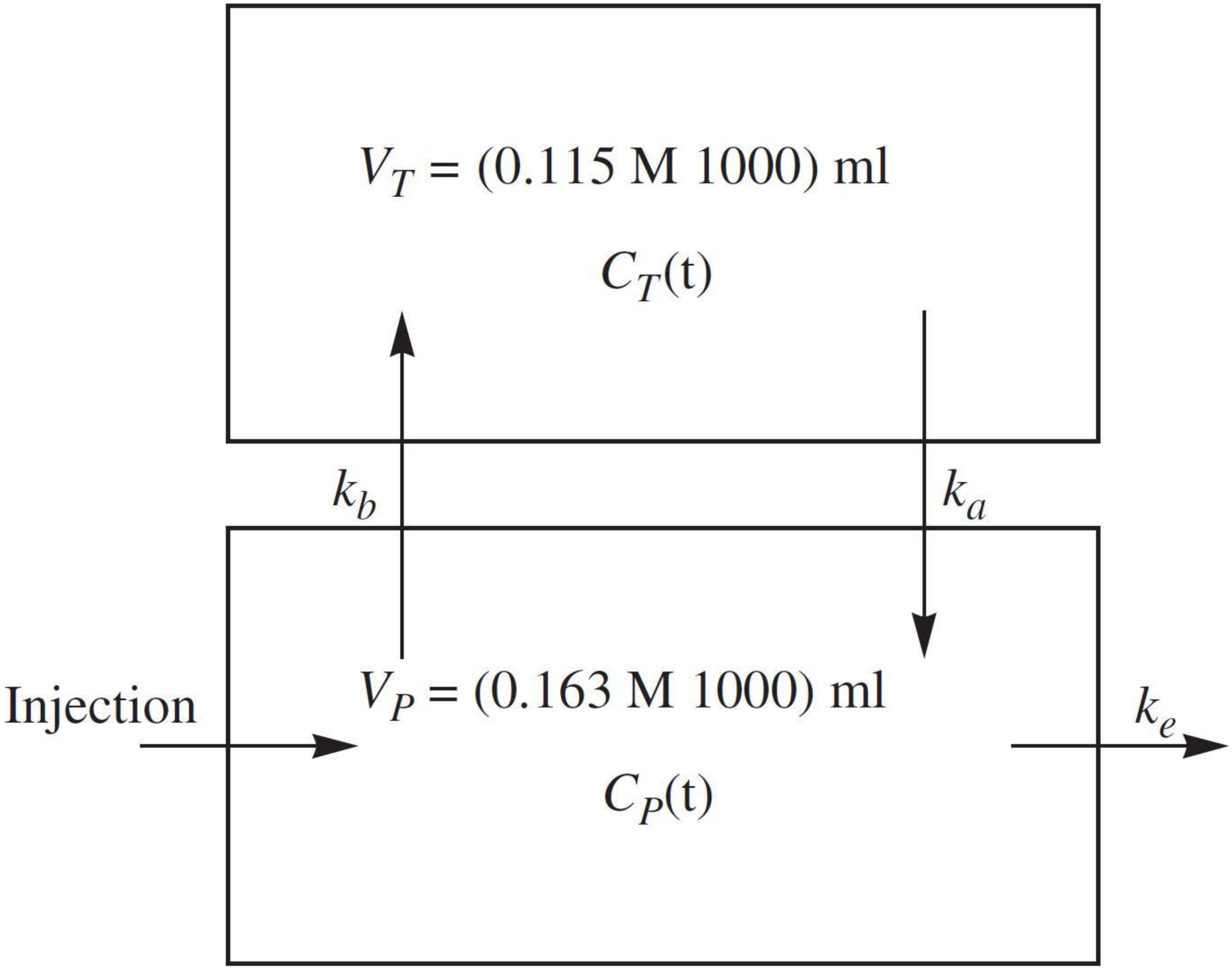
Brian Winkel

Abstract: We describe the use of browsing and searching (in libraries, online, inside sources, at meetings, in abstracts, etc.) as a way to stimulate the teacher of undergraduate mathematics, specifically in differential equations. The approach works in all other areas of mathematics. Browsing can help build new and refreshing teaching materials based on how mathematics is used and explored in places other than mathematics. These "other" places are where almost all of our students will be going after they study with us and we should: (i) know about their journey and arrival points; and (ii) understand the disciplinary approaches for those areas which sent these students to us in the first place for their mathematics studies. We describe a personal browsing experience that spanned almost 40 years and proved to be very worthwhile in finding applications of differential equations to modeling Lysergic Acid Diethylamide in the human body.

Keywords: Browsing and searching, sources, mathematical modeling, differential equations, compartment model, pharmacokinetics, Lysergic Acid Diethylamide (LSD).

	Time (hr)	0.833	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

Table 1. Summary of data collected [1, 14] on 5 male volunteers who were administered LSD and then tested on performance (Perform Score (%)) on simple addition questions. Both performance Score and Plasma Concentrations of LSD were recorded at 5, 15, 30, 60, 120, 240, and 480 minutes after the initial infusion of LSD.


V_T = (0.115 M 1000) ml
C_T(t)
k_b
k_a
Injection
V_P = (0.163 M 1000) ml
C_P(t)
k_e

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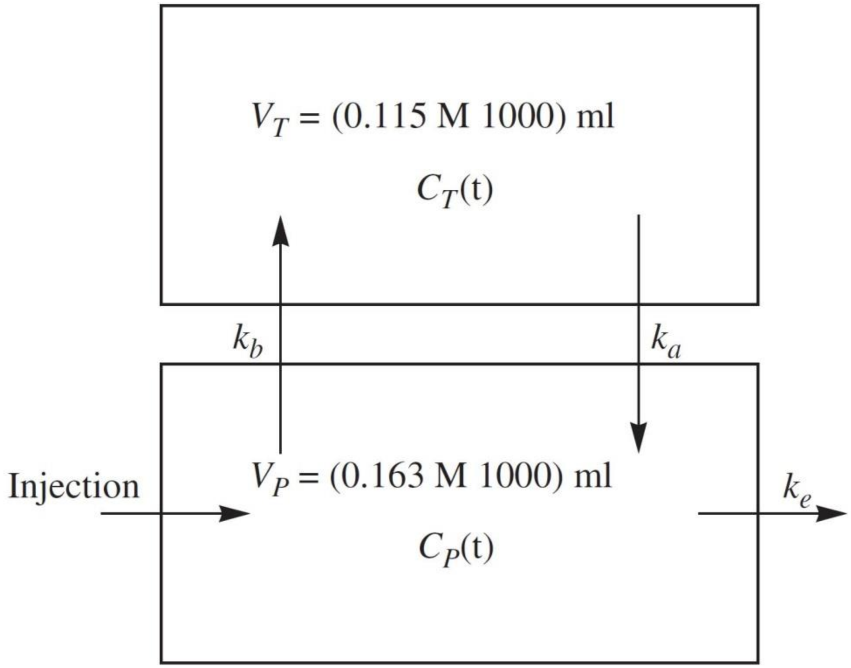


Compartment model

Pharmacokinetics

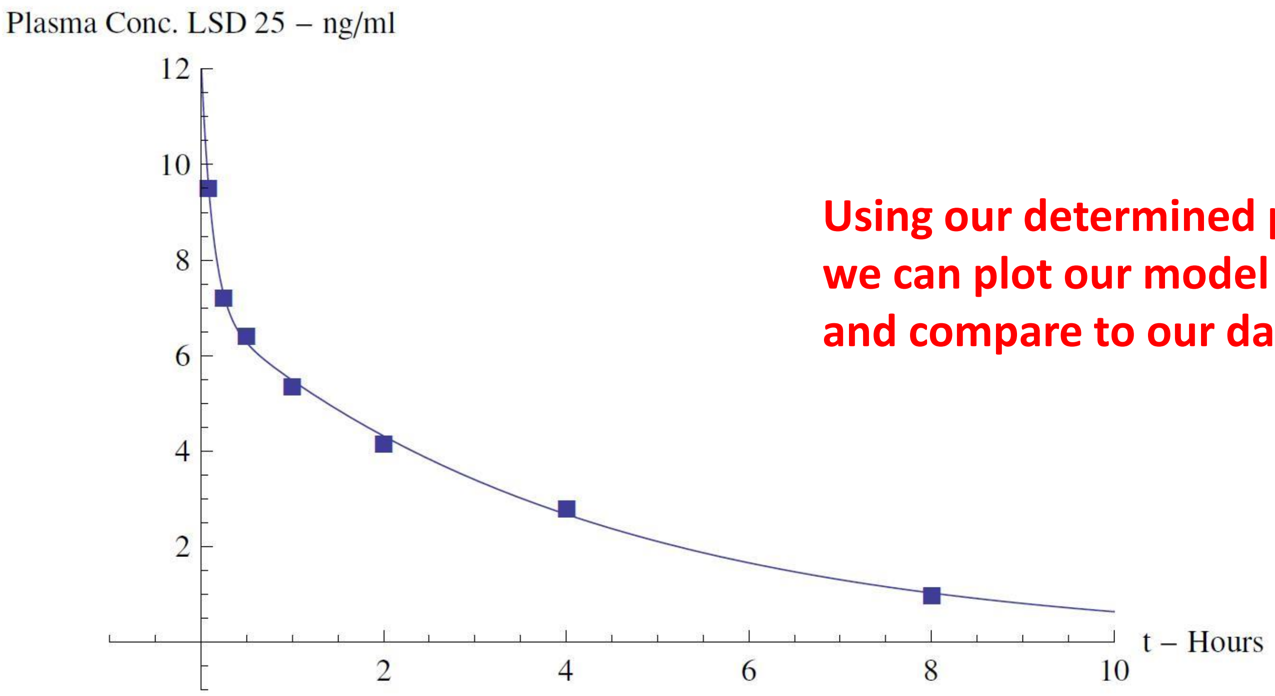
Model building

$$
\begin{aligned}
V_P C_P'(t) &= k_a V_T C_T(t) - k_b V_P C_P(t) - k_e V_P C_P(t) \\
V_T C_T'(t) &= k_b V_P C_P(t) - k_a V_T C_T(t) \,.
\end{aligned}
$$

$$V_P C_P'(t) = k_a V_T C_T(t) - k_b V_P C_P(t) - k_e V_P C_P(t)$$
$$V_T C_T'(t) = k_b V_P C_P(t) - k_a V_T C_T(t)\,.$$

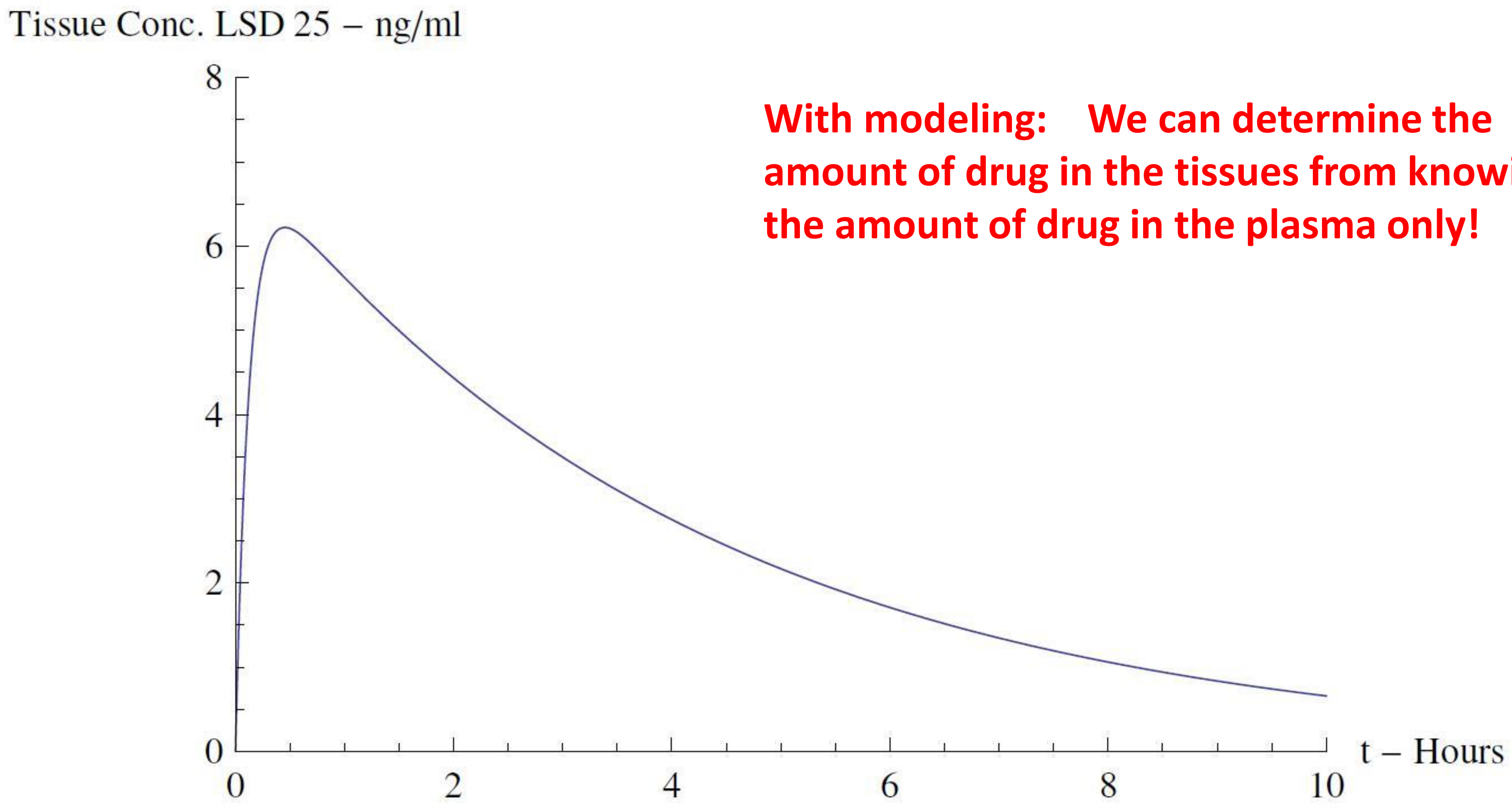
Solve with parameters and use data to form the sum of square errors. Then minimize SSE in terms of parameters.

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

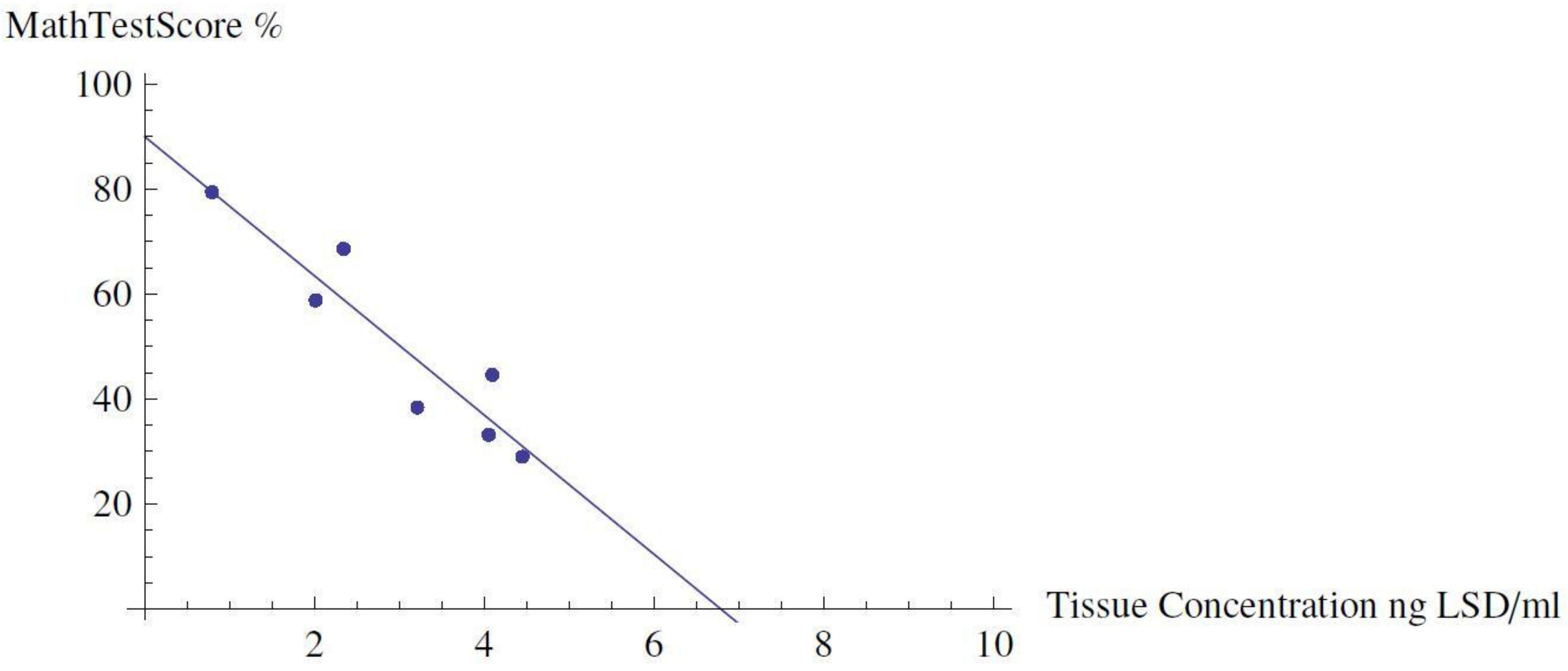


Using our determined parameters we can plot our model prediction and compare to our data. Not bad!

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



With modeling: We can determine the amount of drug in the tissues from knowing the amount of drug in the plasma only!


MathTestScore %
100
80
60
40
20
2
4
6
8
10
Tissue Concentration ng LSD/ml

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Reaching out to local industry colleagues . . . .

. . . led to three hour workshop by chemist and mathematician from The Upjohn Company on pharmacokinetics.

Brought STEM faculty AND students together for active learning, working session on modeling and parameter estimation

Metzler, C. M. 1969. A mathematical model for the pharmacokinetics of LSD effect. *Clinical Pharmacology and Therapeutics*. 10(5): 737–740.

Metzler, C. M. and G. L. Elfring. 1978. Letter to the Editor: Curve fitting and modeling in pharmacokinetics: a response. *Journal of Pharmacokinetics and Pharmacodynamcs*. 6(5): 443–446.

Resources: Potential Scenario Ideas

Start a new Potential Scenario Idea

Type: Potential Scenario Ideas Go

Tag	Resources Sort by Title	Info
[All]	1935Gause Experimental Demonstration...	Select a resource to see details.
absorption (3)	1935Gause Paramecia-Yeast...	
absorption rate (1)	1957 Axelrod Et Al Distribution And...	
acceleration (1)	1964-AghananianBing-Persistence Of...	
accelerometer (1)	1966IntriligatorBrito-Predator-Prey...	
accumulative advantage (1)	1967-Isrealsson...	
advection (1)	1967Wagner Computers in pharmacokinetics	
advection-reaction equations (1)	1968WagnerEtAl Performance Test...	
advertising (1)	1969-JohnssonIsraelsson-Phase Shift...	
aerodynamic drag (1)	1969MetzlerMathModelOfLSD	
age (1)	1971-BoyesEtal-Lidocaine In Man	
age-structure (1)	1971-Metzler-Usefulness Of Two...	
agent-based (4)	1975-Burghes-PopulationDynamics	
AIDS epidemic (1)	1975-Griffel-FormationSolutionDEModels	

Top Rated

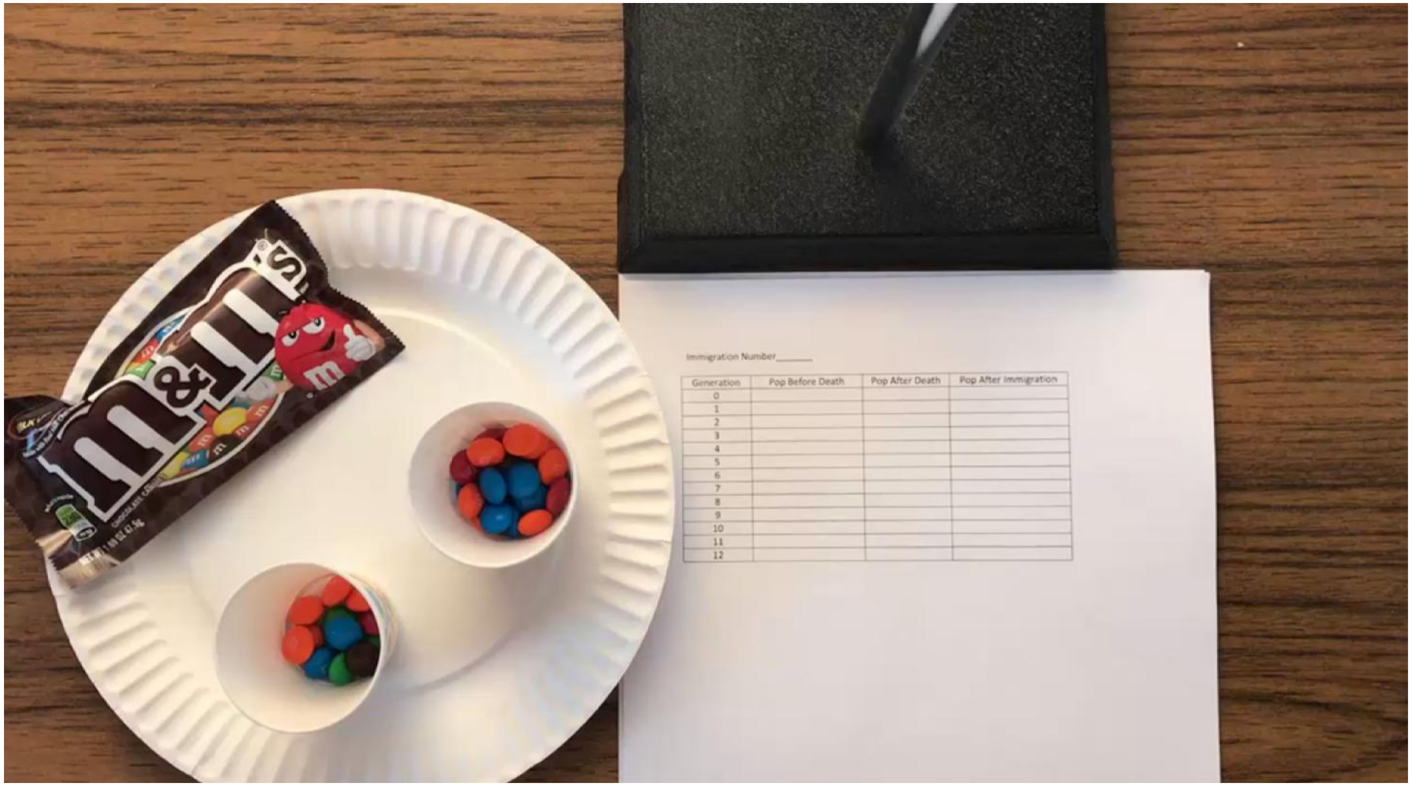
The following are top-rated resources of this type.

1935Gause Paramecia-Yeast Predator-Prey-G.F.Gause Study

20 Jun 2015 | Potential Scenario Ideas | Contributor(s): G. F. Gause

This is the classic paper, Experimental Demonstration of Volterra's Periodic Oscillations in the Numbers of Animals in the Journal of Experimental Biology by G. F. Gause from pp.44-48.Data in a plot is offered on paramecia (predator) and yeast (prey) through several cycles. Parameter...

Death and Immigration with m&ms – a first day Modeling Scenario



Build a mathematical model of this death and immigration

Collect data.

Which first? Concurrent?

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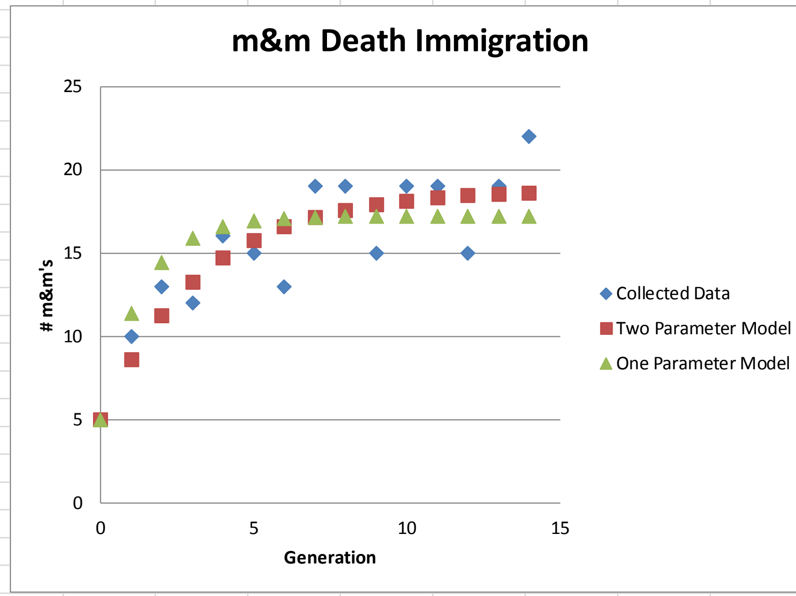
Prepared by Brian Winkel, Director SIMIODE, 21 January 2017

Using Solver to estimate parameters a and b in model **M(n+1) = a*M(n) + b, M(0) = 5.**
We estimate first two parameters a and b and then only parameter a with parameter b set to 10 (known).

Initial Population 5 **Immigration** 9
Parameters

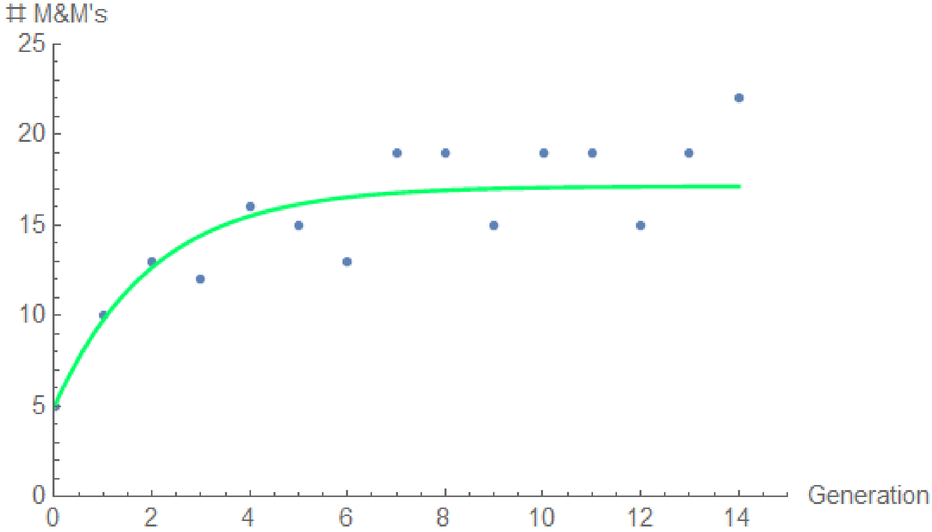
Using Solver to estimate parameters a and b in model M(n+1) = a*M(n) + b, M(0) = 50.
We estimate first two parameters a and b and then only parameter a with parameter b set to 9 (known).

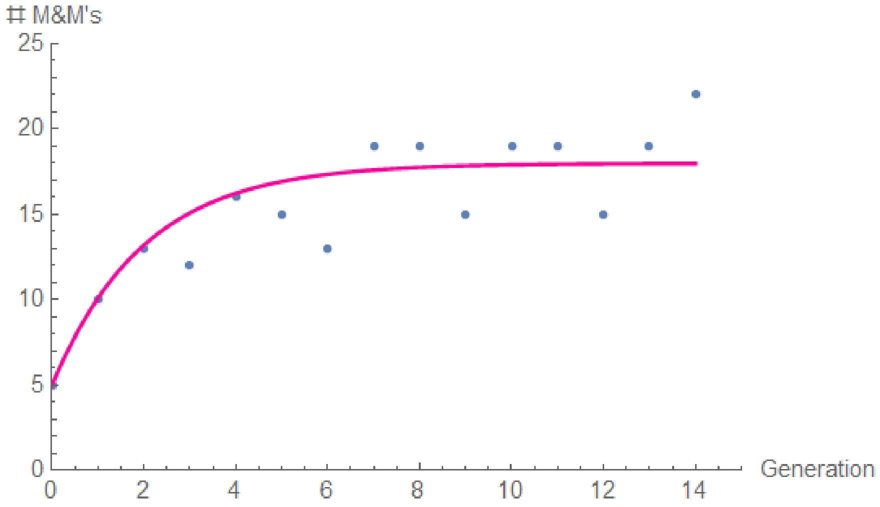
		a =	0.738900705		a =	0.477462		a =	0.5
		b =	4.907756759		b =	9	<--Fixed	b =	9
		Two	**Two**		**One**	**One**		**Ideal**	**Ideal**
	Obs.	**Parameter**	**Parameter**		**Parameter**	**Parameter**		**Model**	**Model**
Time	**Pop**	**Model**	**Diff^2**		**Model**	**Diff^2**			**Diff^2**
0	5	5	0		5	0		5	0
1	10	8.602	1.954		11.387	1.925		11.500	2.250
2	13	11.264	3.014		14.437	2.065		14.750	3.063
3	12	13.231	1.515		15.893	15.156		16.375	19.141
4	16	14.684	1.732		16.588	0.346		17.188	1.410
5	15	15.758	0.574		16.920	3.688		17.594	6.728
6	13	16.551	12.611		17.079	16.637		17.797	23.010
7	19	17.137	3.469		17.154	3.406		17.898	1.213
8	19	17.571	2.043		17.191	3.274		17.949	1.104
9	15	17.891	8.356		17.208	4.875		17.975	8.848
10	19	18.127	0.762		17.216	3.182		17.987	1.026
11	19	18.302	0.487		17.220	3.168		17.994	1.013
12	15	18.431	11.772		17.222	4.937		17.997	8.981
13	19	18.526	0.224		17.223	3.158		17.998	1.003
14	22	18.597	11.580		17.223	22.817		17.999	16.006
		SSError	60.093		**SSError**	88.634		**SSError**	94.795



Using Solver to minimize the Sum of Square Errors
in each case where first in two parameter estimate
a and b are being estimated and second in one parameter
estimate where only a is being estimated with b known.

Using differential equation model
$m'(t) = -a\, m(t) + b, \quad m(0) = 5$.





Using sum of square errors - Mathematica

Estimating only b, b = 8.58

Estimating a and b, a = 0.37 and b = 6.62

Dina Yagodich, Frederick Community College,

A memorable quote from a student evaluation from that semester answered the question "What class assignment or activity did you find to be the most useful?" with the following:

> ***Believe it or not, the M&M activity on the first day of class really stood out to me. It helped to show the real world applications of Differential Equations and I thought it was amazing that we could build an equation using real world data.***

Even if no other modeling is done the rest of the semester, **starting a class with a modeling activity such as this paints a clear picture on the types of problems differential equations can be used to solve,** demonstrates the modeling cycle, and introduces numerical solution methods.

The M&Ms activity on my first day of DiffEq was a success.

I didn’t realize how useful it was going to be in following classes.

I now have a metaphor for initial conditions ("Remember, that was our Generation Zero of M&Ms"), I already have a differential equation that they can solve both as separable and as linear, etc.

I thought of it more as a "get their feet wet" type of activity, but really it turned into a bigger part of my first week.

Marko Budišić, Clarkson University, 30 September 2017

Richard Corban Harwood 5:56 am 22 Jan 2017

Great project idea and thanks for the video!

I tried a similar, but shorter, version on Day 1 this semester. This was a great way to learn student names day one. Note: I had a class of 18 and a class of 28 for this.

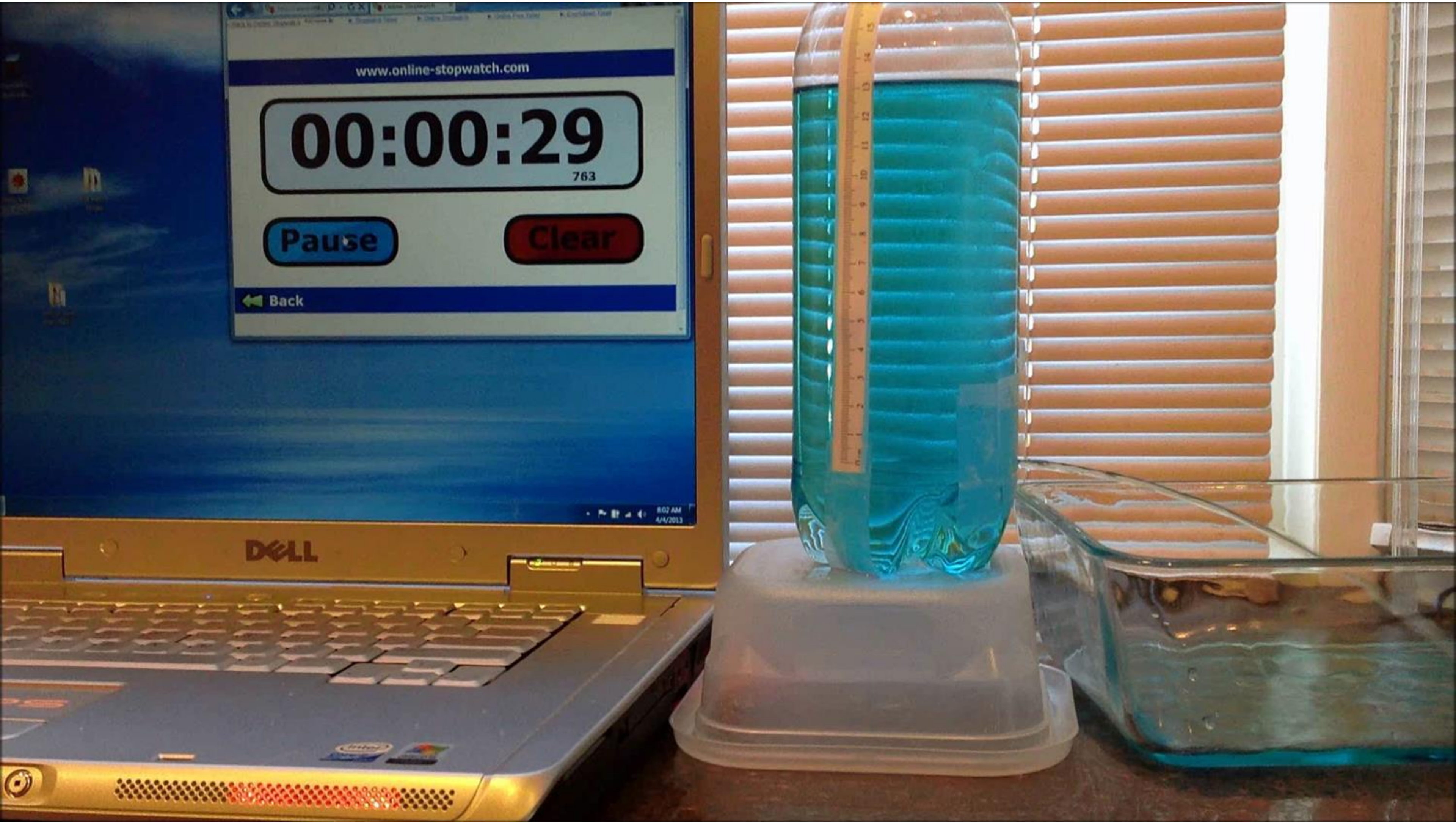
1) I told the class what we would do (roll m&m's eat about half of them, add 1, and repeat) and had them pair up, introduce themselves to each other and write down a prediction for the number of m&m's at the end of the class list.

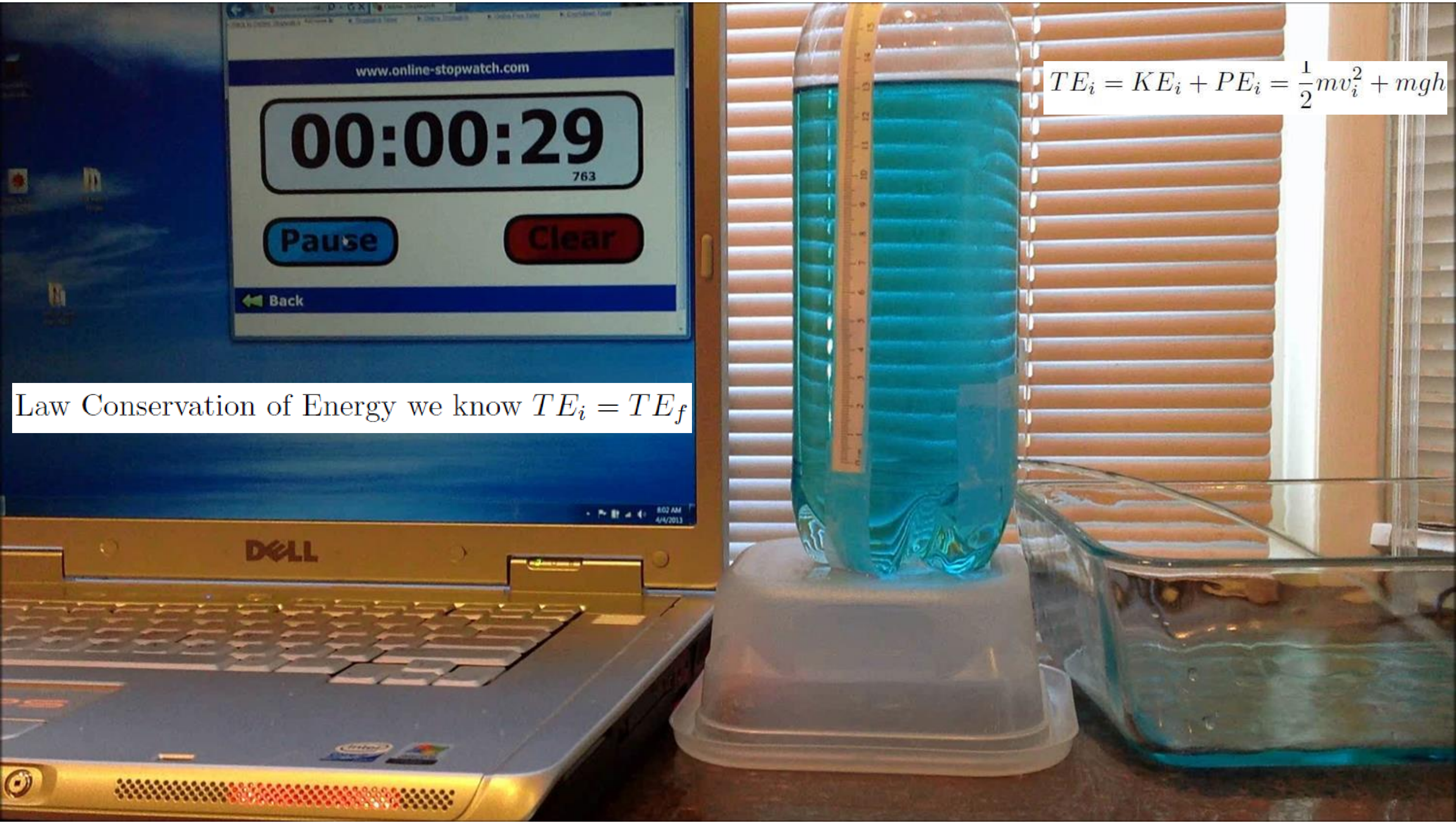
2) Calling on the first 10 students on my class list, I handed them each 1 m&m. They each rolled it and if it came up with an M, (died) they got to eat it. Then I handed out 1 m&m to the next student on my class list and had everyone with an m&m raise their hand so I could tally the total on a spreadsheet (projected onto a screen).

3) I plotted the data on the spreadsheet and we had a good discussion about why most of them predicted 0 or 1 (though it ended around 2 for both classes).

4) Then I guided the class in setting up a differential equation model, x'=1-x/2, verified its solution (which I provided) and checked the end behavior as t->infinity. Then we looked at the equilibrium point and compared it to their predictions.

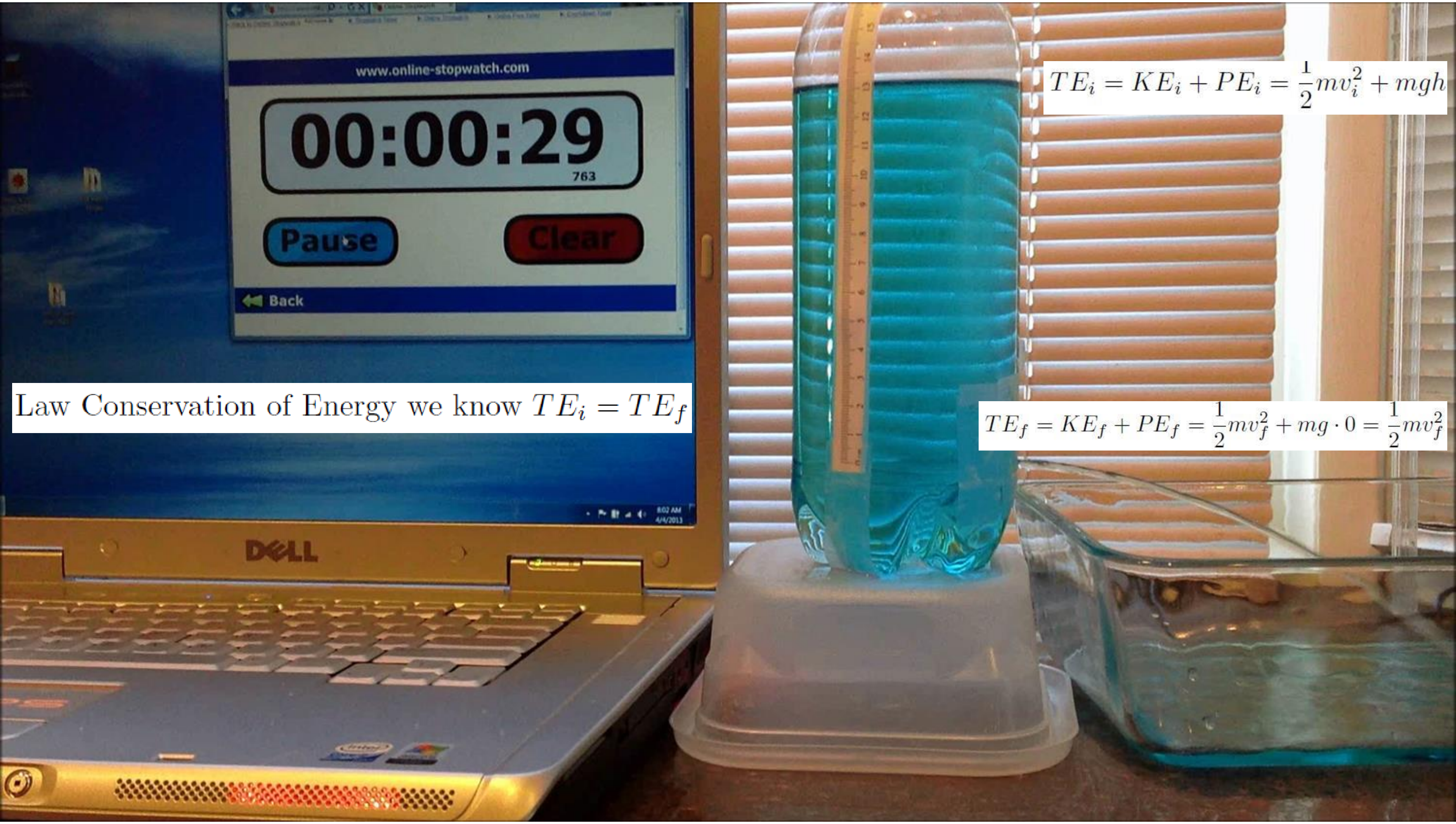
This was a helpful way to introduce the idea of the course, get to know them and warm them up for a two week group project starting the next class day. I chose to follow this M&M modeling scenario with the modeling scenario: Simulating the spread of the Common Cold.


www.online-stopwatch.com
00:00:29
763
Pause
Clear
Back
DELL



$TE_i = KE_i + PE_i = \frac{1}{2}mv_i^2 + mgh$

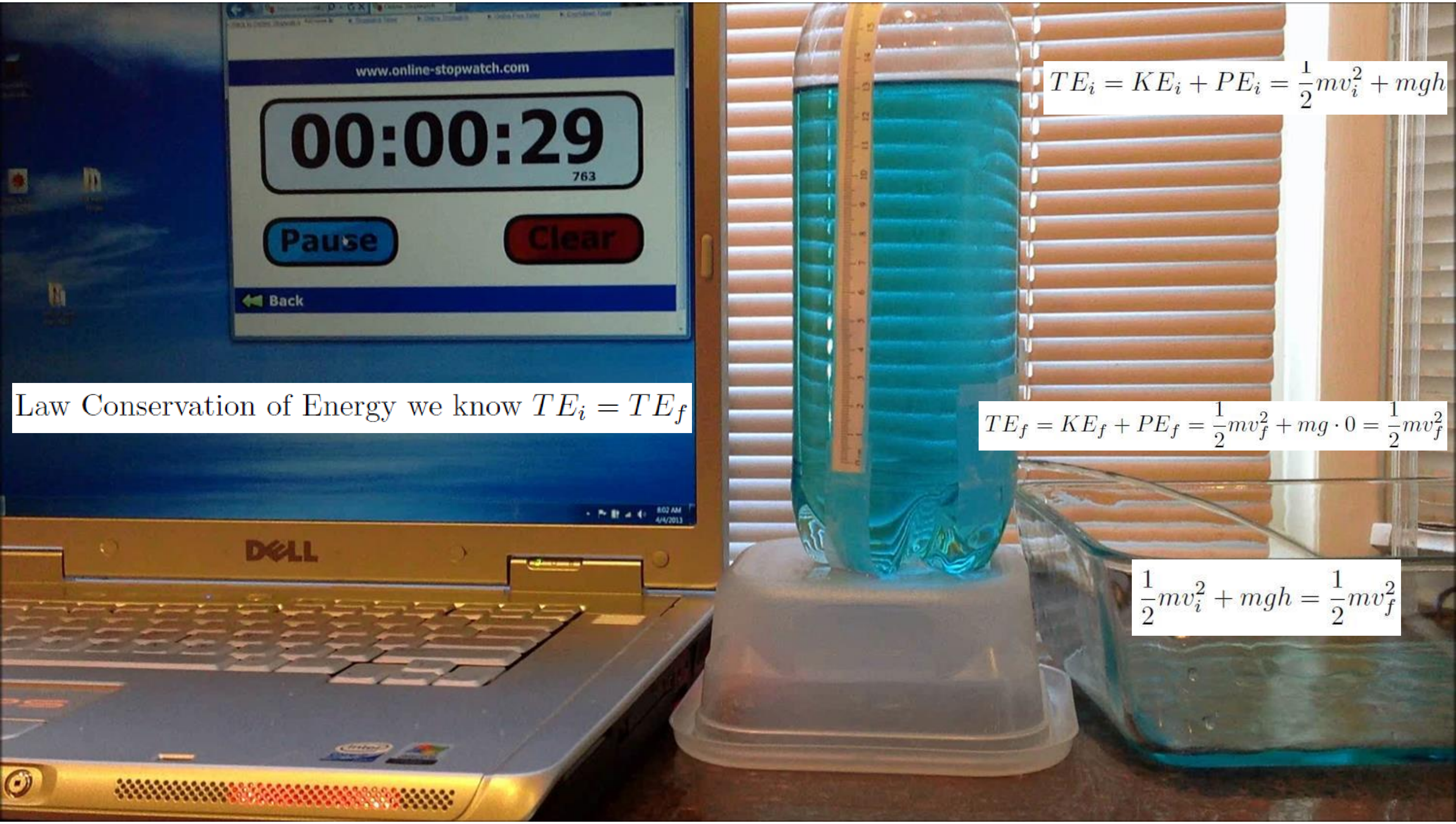
Law Conservation of Energy we know $TE_i = TE_f$



$$TE_i = KE_i + PE_i = \frac{1}{2}mv_i^2 + mgh$$

Law Conservation of Energy we know $TE_i = TE_f$

$$TE_f = KE_f + PE_f = \frac{1}{2}mv_f^2 + mg \cdot 0 = \frac{1}{2}mv_f^2$$

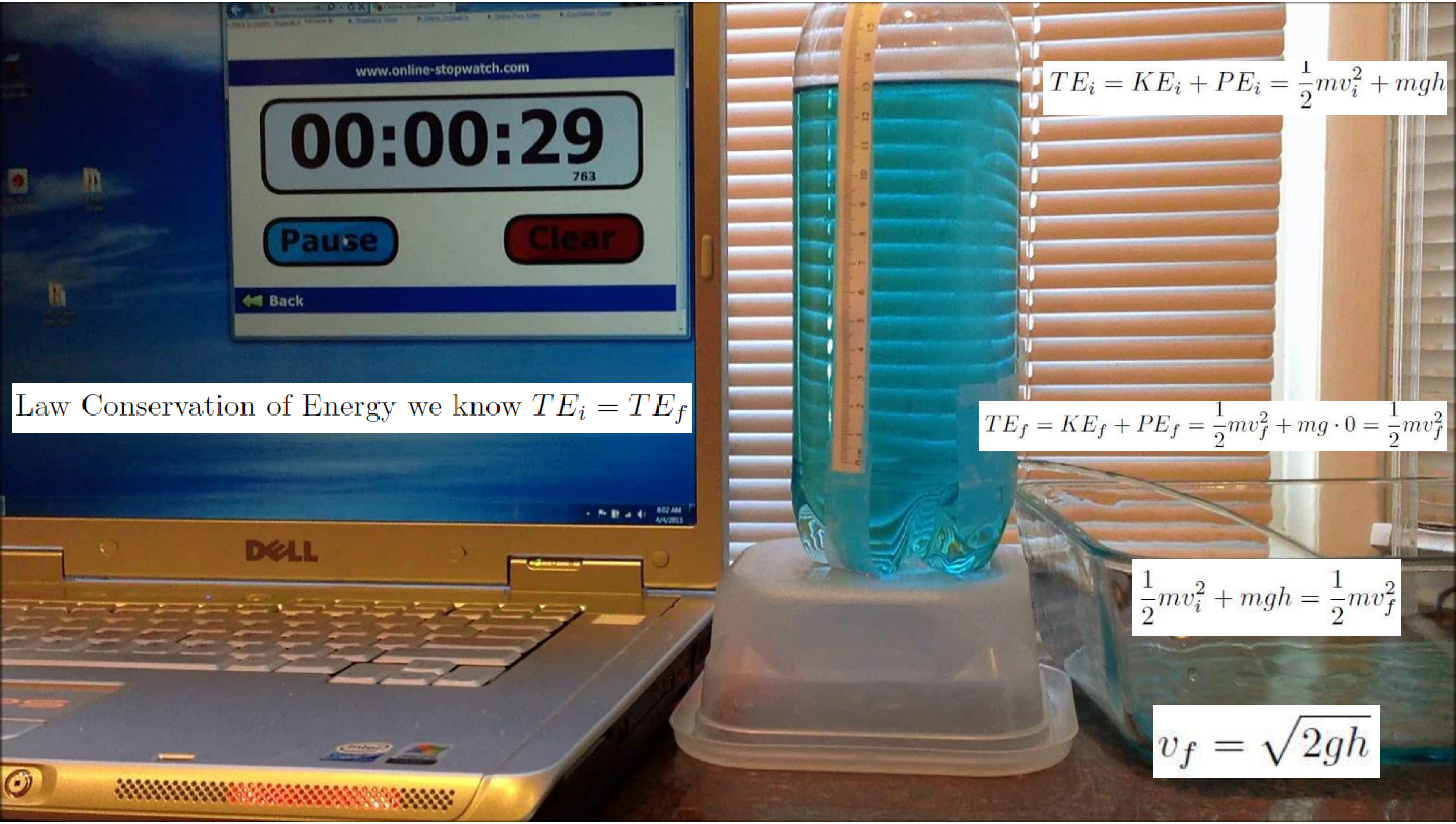


$$TE_i = KE_i + PE_i = \frac{1}{2}mv_i^2 + mgh$$

Law Conservation of Energy we know $TE_i = TE_f$

$$TE_f = KE_f + PE_f = \frac{1}{2}mv_f^2 + mg \cdot 0 = \frac{1}{2}mv_f^2$$

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



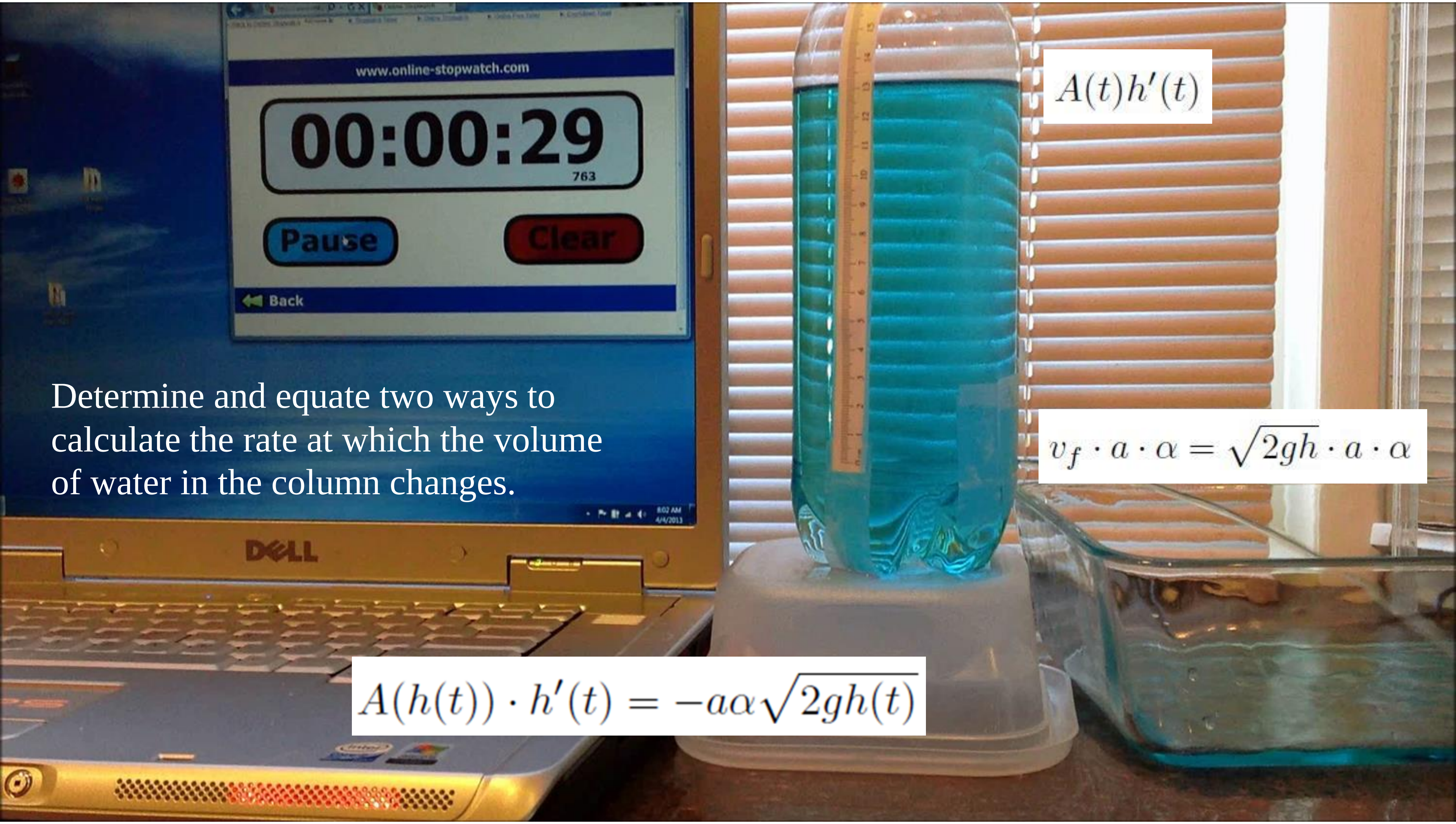
Law Conservation of Energy we know $TE_i = TE_f$

$$TE_i = KE_i + PE_i = \frac{1}{2}mv_i^2 + mgh$$

$$TE_f = KE_f + PE_f = \frac{1}{2}mv_f^2 + mg \cdot 0 = \frac{1}{2}mv_f^2$$

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

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

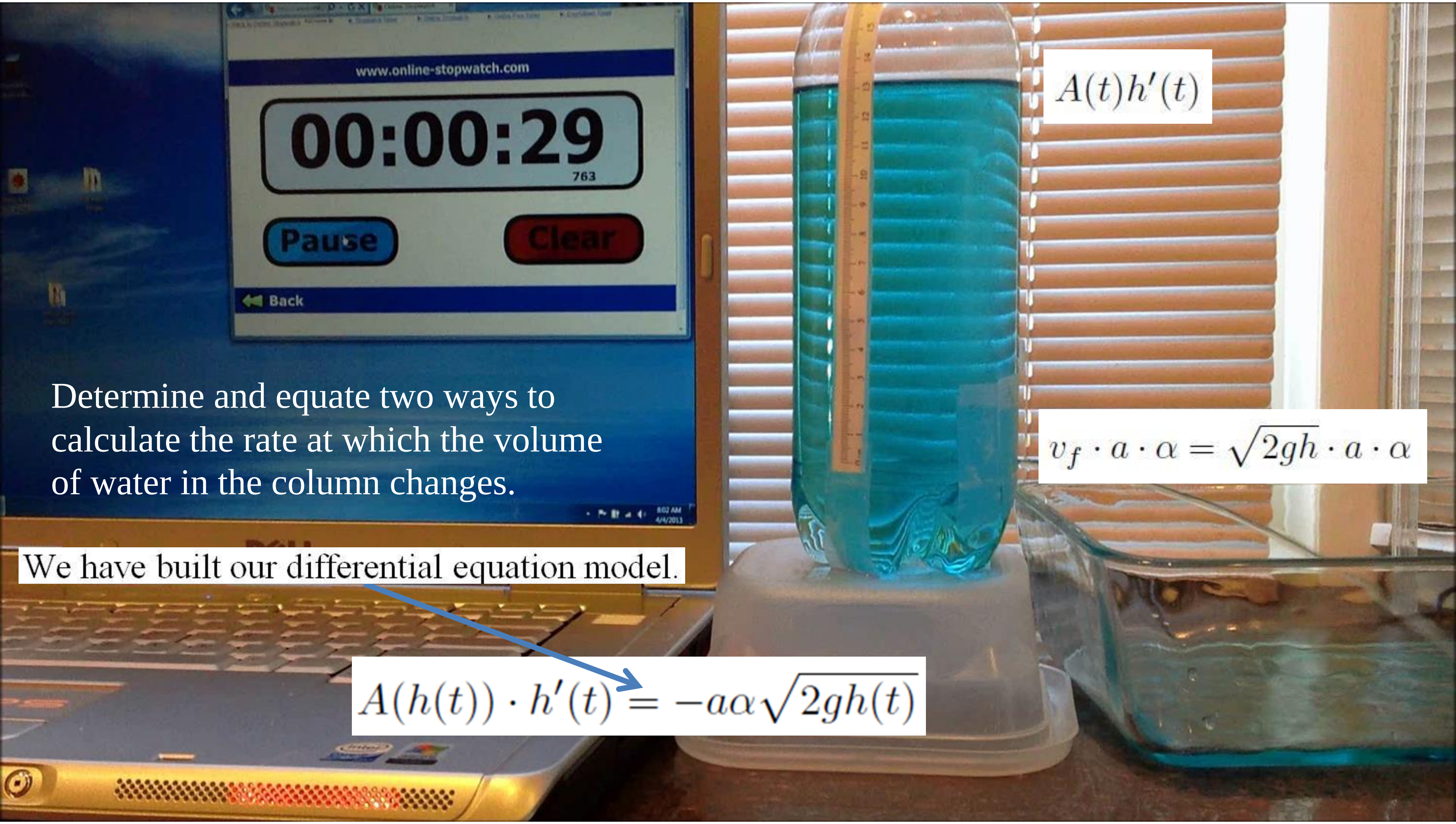


$$A(t)h'(t)$$

$$v_f \cdot a \cdot \alpha = \sqrt{2gh} \cdot a \cdot \alpha$$

Determine and equate two ways to calculate the rate at which the volume of water in the column changes.

$$A(h(t)) \cdot h'(t) = -a\alpha\sqrt{2gh(t)}$$



$A(t)h'(t)$

$v_f \cdot a \cdot \alpha = \sqrt{2gh} \cdot a \cdot \alpha$

Determine and equate two ways to calculate the rate at which the volume of water in the column changes.

We have built our differential equation model.

$$A(h(t)) \cdot h'(t) = -a\alpha\sqrt{2gh(t)}$$

$$A(h(t)) \cdot h'(t) = -a\alpha\sqrt{2gh(t)}$$

We now solve for *h(t)* and note that *A(h(t))* = *A*, the cross-sectional area, is constant, while gathering all the constants *A*, α, and *a* into one big constant, *b*, leaving out *g*.

This is a differential equation in which we need to recover *h(t)*. It is referred to as *Torricelli's Law.* Evangelista Torricelli, (1608-1647).

$$h'(t) = -b\sqrt{gh(t)}$$

All too often a differential equations course starts here with an "abstract" differential equation and no motivation and the instructor says, "I will now show you how to solve the differential equation using a technique we will call Separation of Variables." And the symbol manipulation begins . . . . Until. Voila!

$$h(t) = \frac{1}{4}\left(b^2gt^2 - 4b\sqrt{gh_0}t + 4h_0\right)$$

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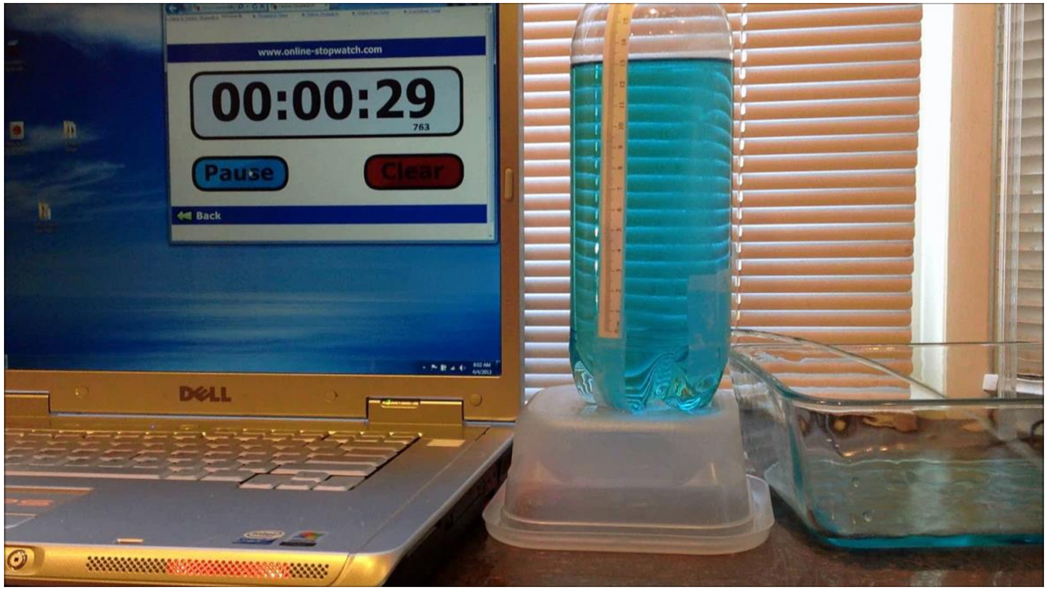
$$h(t) = \frac{1}{4}\left(b^2 g t^2 - 4b\sqrt{g h_0}\, t + 4h_0\right)$$

We still have the problem of estimating the parameter *b*.

For g, the acceleration due to gravity, is known and we could obtain h_0, the initial height of the column of water from the video.

Can we collect data from the video to estimate the parameter *b*?

Sure we can.
AND we do!



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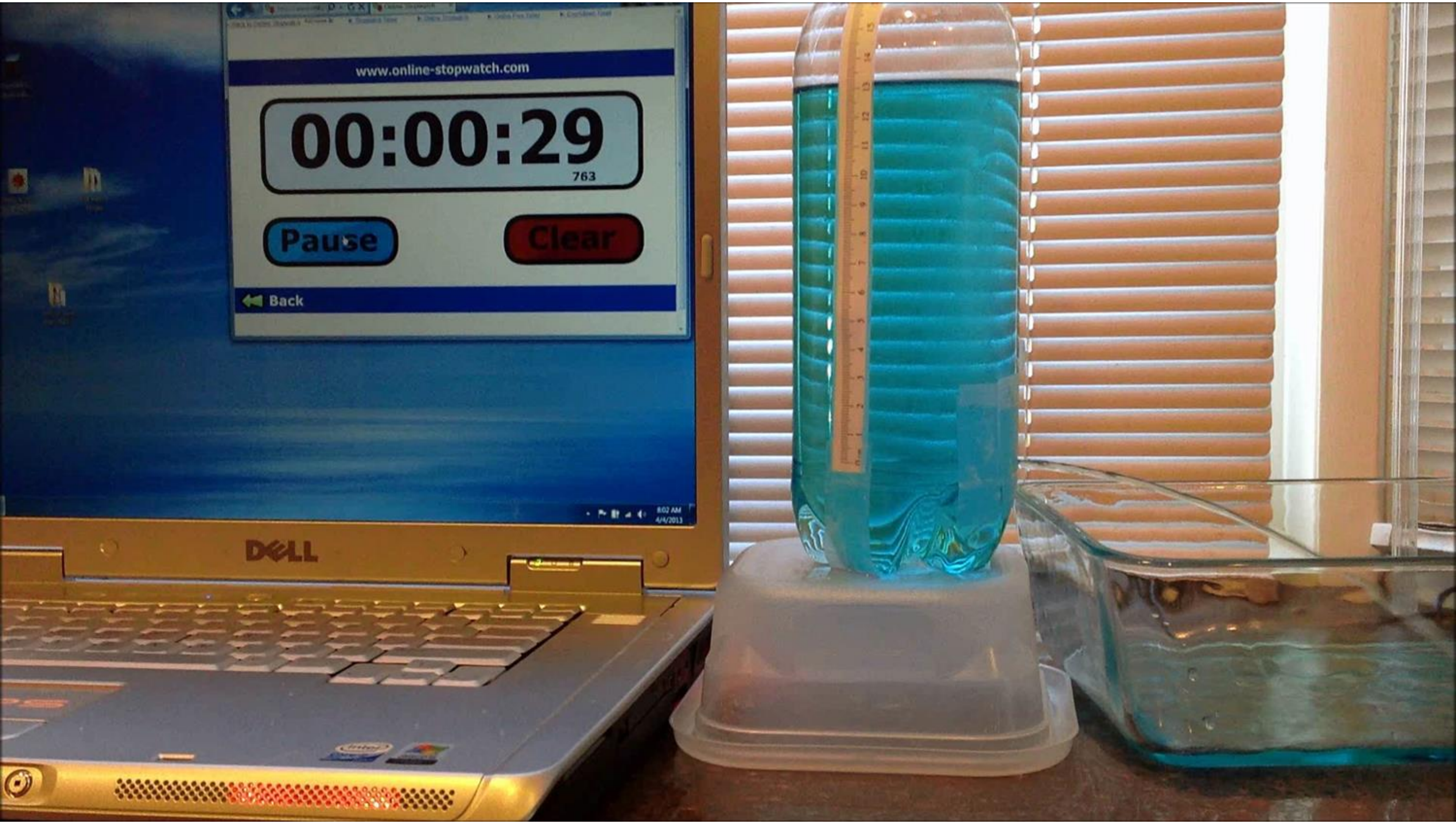

Search SIMIODE YouTube and select video, do 720p/1080p. Stop/start to collect data. OrSearch 9Over64 Inch.

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This is data from another video which we used to estimate the parameter.

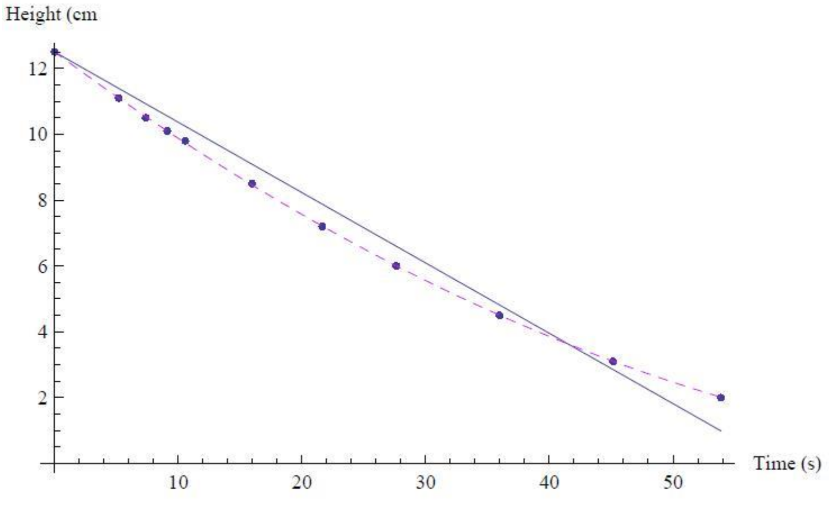
Clock Time t (min)	Relative Time t (s)	Linear h (cm)	Torricelli h (cm)	Observed h (cm)
1:40.419 = 100.419	0	12.5	12.5	12.5
1:45.598 = 105.598	5.179	11.3935	11.1028	11.1
1:47.568 = 107.788	7.369	10.9256	10.5369	10.5
1:49.623 = 109.523	9.104	10.5549	10.0991	10.1
1:50.985 = 110.985	10.566	10.2426	9.7374	9.8
1:56.388 = 116,388	15.969	9.08821	8.45786	8.5
2:02.057 = 122.057	21.638	7.87702	7.21218	7.2
2:08.032 = 128.032	27.613	6.60046	6.00662	6.0
2:16.386 = 136.386	35.967	4.81562	4.50576	4.5
2:25.568 = 145.568	45.149	2.85388	3.10461	3.1
2:34.116 = 154.286	53.867	0.991273	2.01507	2.0

We find the parameter b and hence we compute the column “Torricelli” by minimizing the following quantity:

$$SS_{\mathrm{Error}}(b) = \sum_{i=1}^{11} \left(h(t_i) - \hat{h}_i\right)^2$$

Finally we plot our model – purple dashes over our data.

Oh and, of course, we throw in the proverbial linear model to show it is of no use in this case.



This parameter was actually the product of two constants, $a\alpha$, in our model where a was the cross sectional area of the bore hole at the bottom.

α, is important and is called the ***discharge or contraction coefficient***, describing the percentage of the maximum rate at which the water exists the container.

In this case we obtained $\alpha = 0.67$ which is reasonable value compared to other sources.

$$A(h(t)) \cdot h'(t) = -a\alpha\sqrt{2gh(t)}$$

Examples of Tuned Mass Dampers

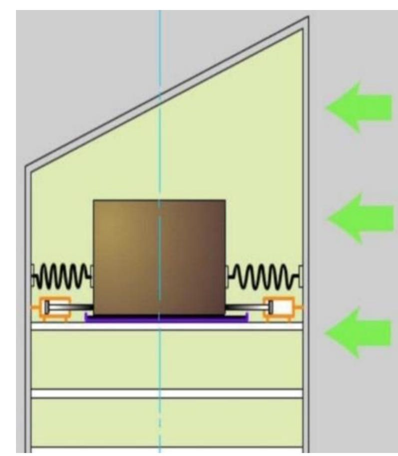
TMD: Schwedter Strasse, Berlin

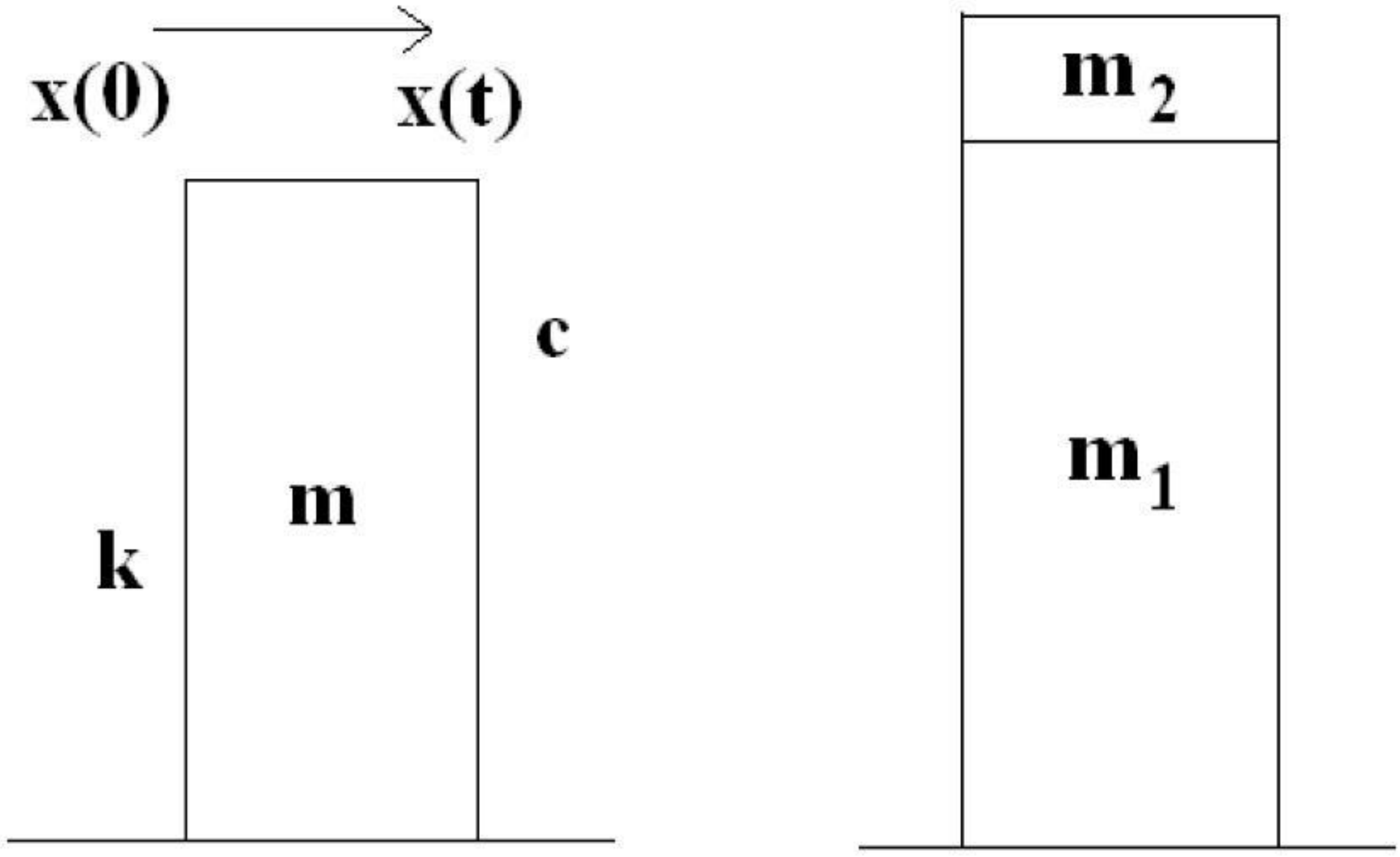
TMD: Skywalk @ Grand Canyon

TMD: Stockbridge Damper

TMD: Taipei 101

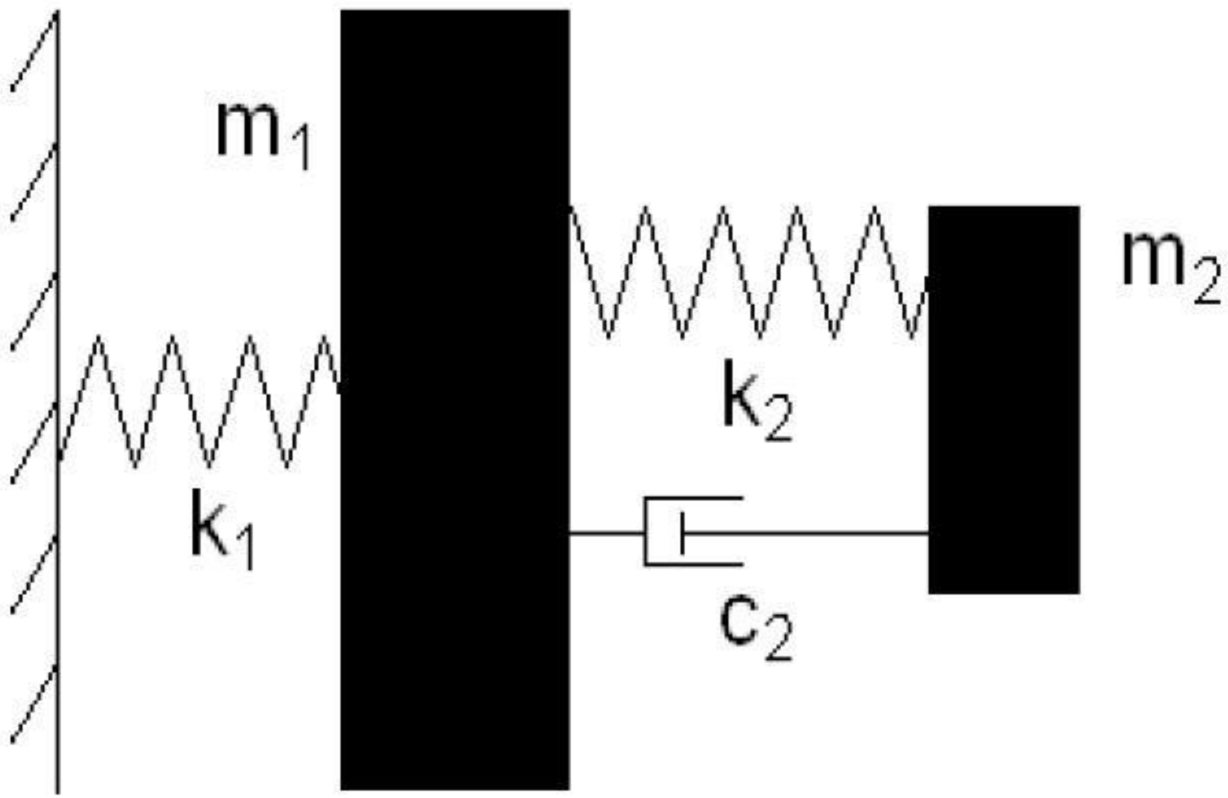
TMD: Citicorp Building





Structure sways? Introduce second mass, but tune it.

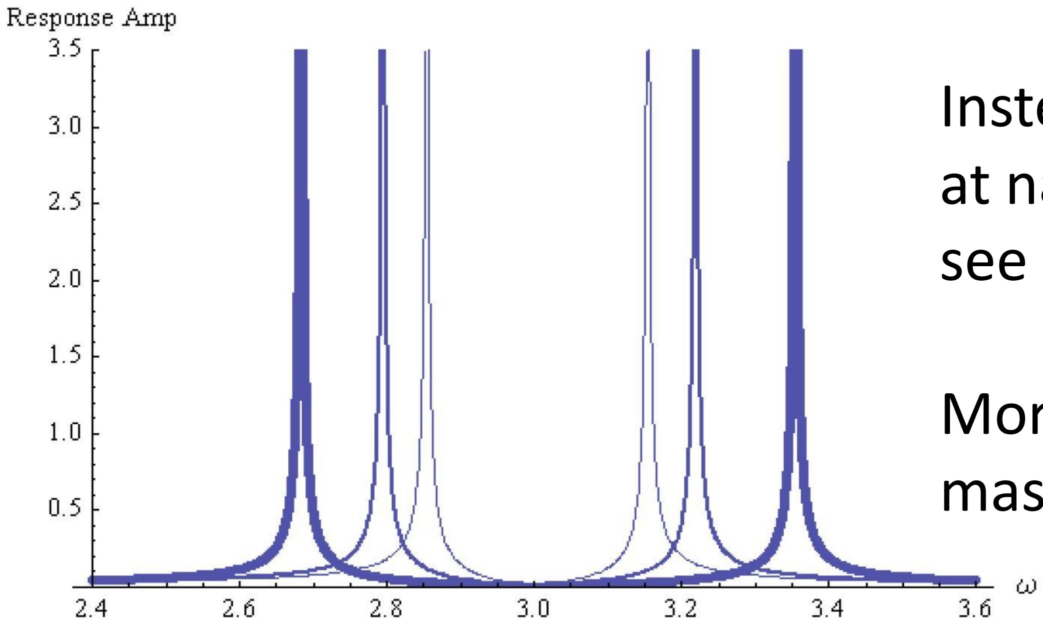
We could analyze more realistic models with resistance to one or both masses.



We build a system of differential equations using FBD for displacement of each mass.

$$m_1 x_1''(t) + k_1 x_1(t) + k_2 x_1(t) - k_2 x_2(t) = F_0 \cos(\omega t),$$

$$m_2 x_2''(t) - k_2 x_1(t) + k_2 x_2(t) = 0\,.$$



Instead of possible resonance at natural frequency ω = 3 we see total damping.

Moreover, the bigger second mass is the wider the coverage.

Time (s)	0	0.347	0.47	0.519	0.582	0.65	0.674	0.717	0.766	0.823	0.87	1.031	1.193	1.354	1.501	1.726	1.873
Distance (m)	0	0.61	1.00	1.22	1.52	1.83	2.00	2.13	2.44	2.74	3.00	4.00	5.00	6.00	7.00	8.50	9.50

Table 1. Time and distance traveled data on a free falling shuttlecock which is dropped from a height of 2 m at rest.

Source: Peastrel, M., R.Lynch, and A. Armenti, Jr. 1980. Terminal velocity of a shuttlecock in vertical fall. *American Journal of Physics*. 48(7): 511-513.

Many sources on falling body with resistance. Use some with real data or generate the real data with students.

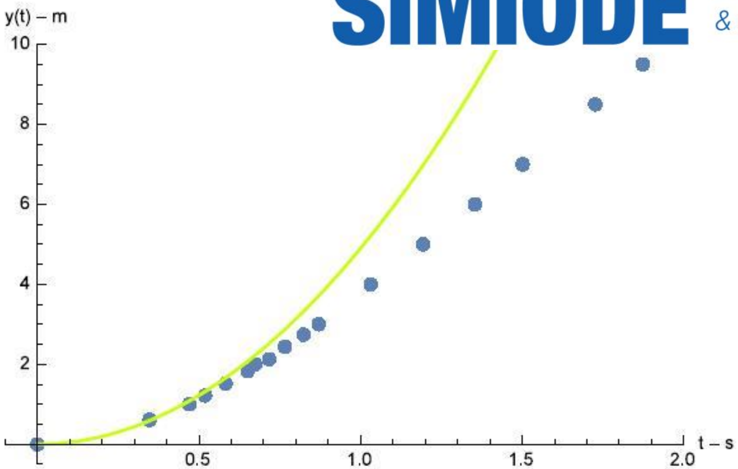


Figure 3. Plot of the model with no resistance, $m * v'(t) = m * g$, and the original data.

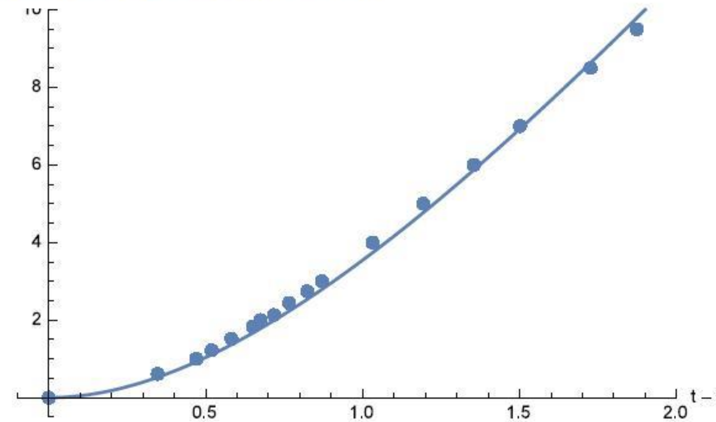


Figure 4. Plot of the model with resistance using $r = 1$, $v'(t) = -k * v(t)^1 + g$, and the original data.

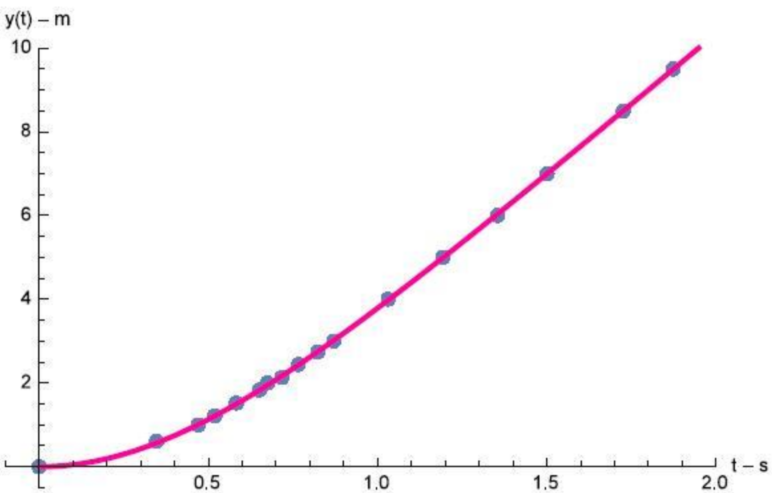


Figure 6. Plot of the model with resistance using $r = 2$, $v'(t) = -k * v(t)^2 + g$, and the original data.

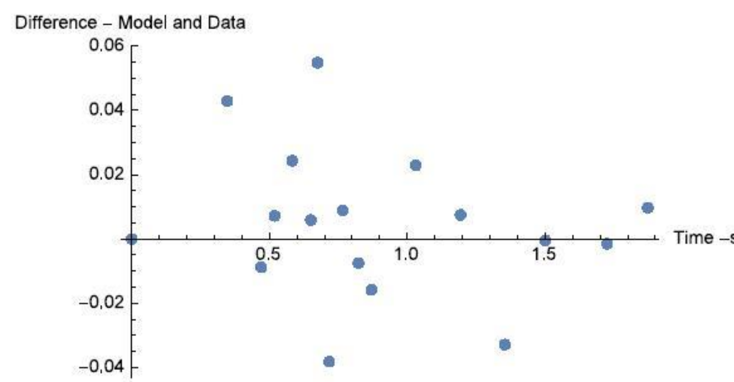


Figure 7. Plot of the residuals(differences between model and data) from the model with resistance using $r = 2$, $v'(t) = -k * v(t)^2 + g$, and the original data.

Model	r	$k = a$	SSE	AIC	
Source	2		0.00920356	**-123.811**	
No Resistance		0	128.369	128.369	
Case	$r = 1$	1	1.06174	0.523775	-55.1584
Case	$r = 2$	2	0.211834	0.00920356	**-123.863**
General r	2.019	.0205	0.00919924	**-121.871**	

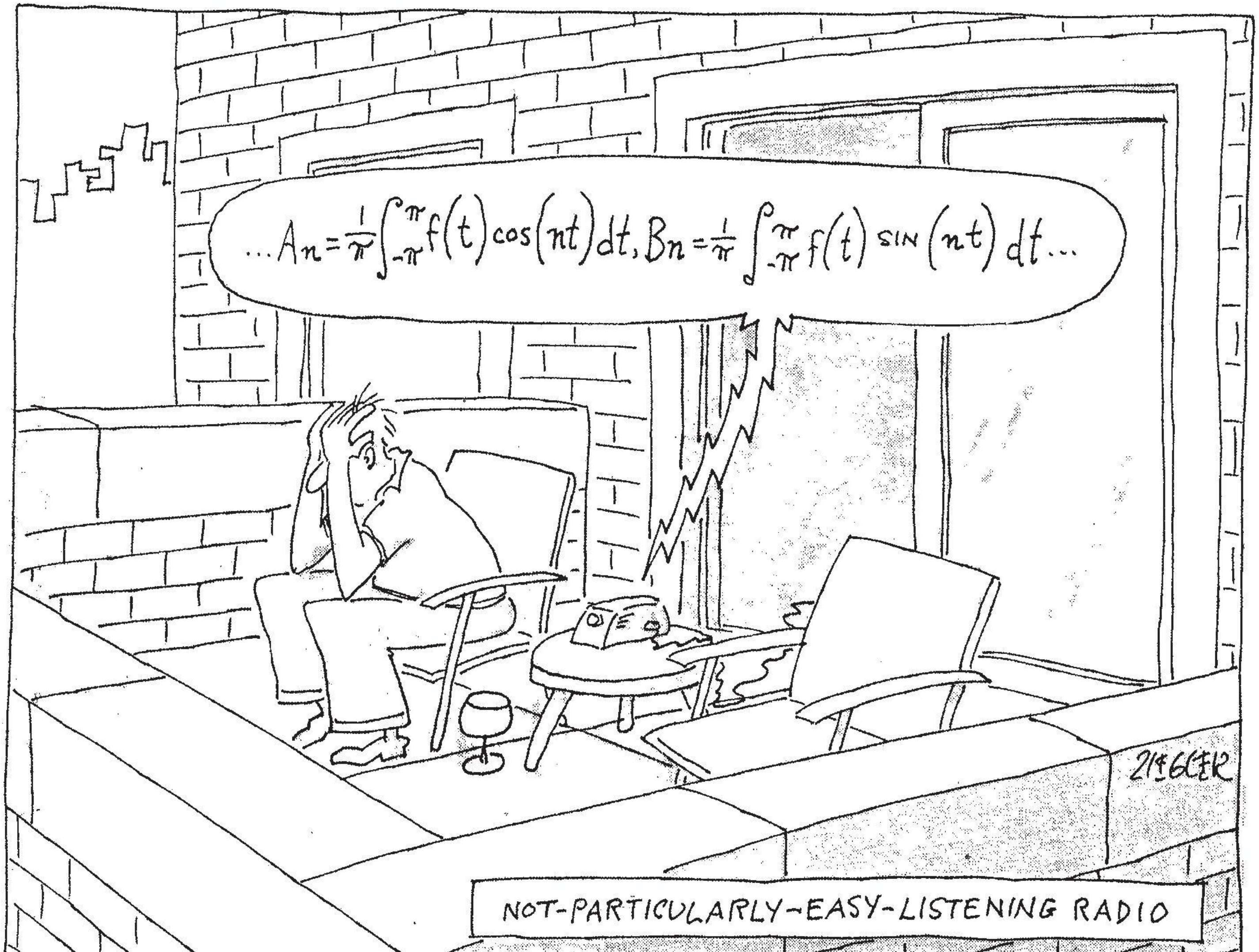
Table 2. Information we need about our models to decide which model is best is presented.

$$AIC = 2(1+k) + n \log\left(\frac{\text{RSS}}{n}\right).$$

k is # parameters and
n is # data points

Akaike information criterion (AIC)

Not all work. . . not all fun. . . building for modeling-first differential equations



These images are related!

$$\sum_{n=0}^{\infty} A_n$$

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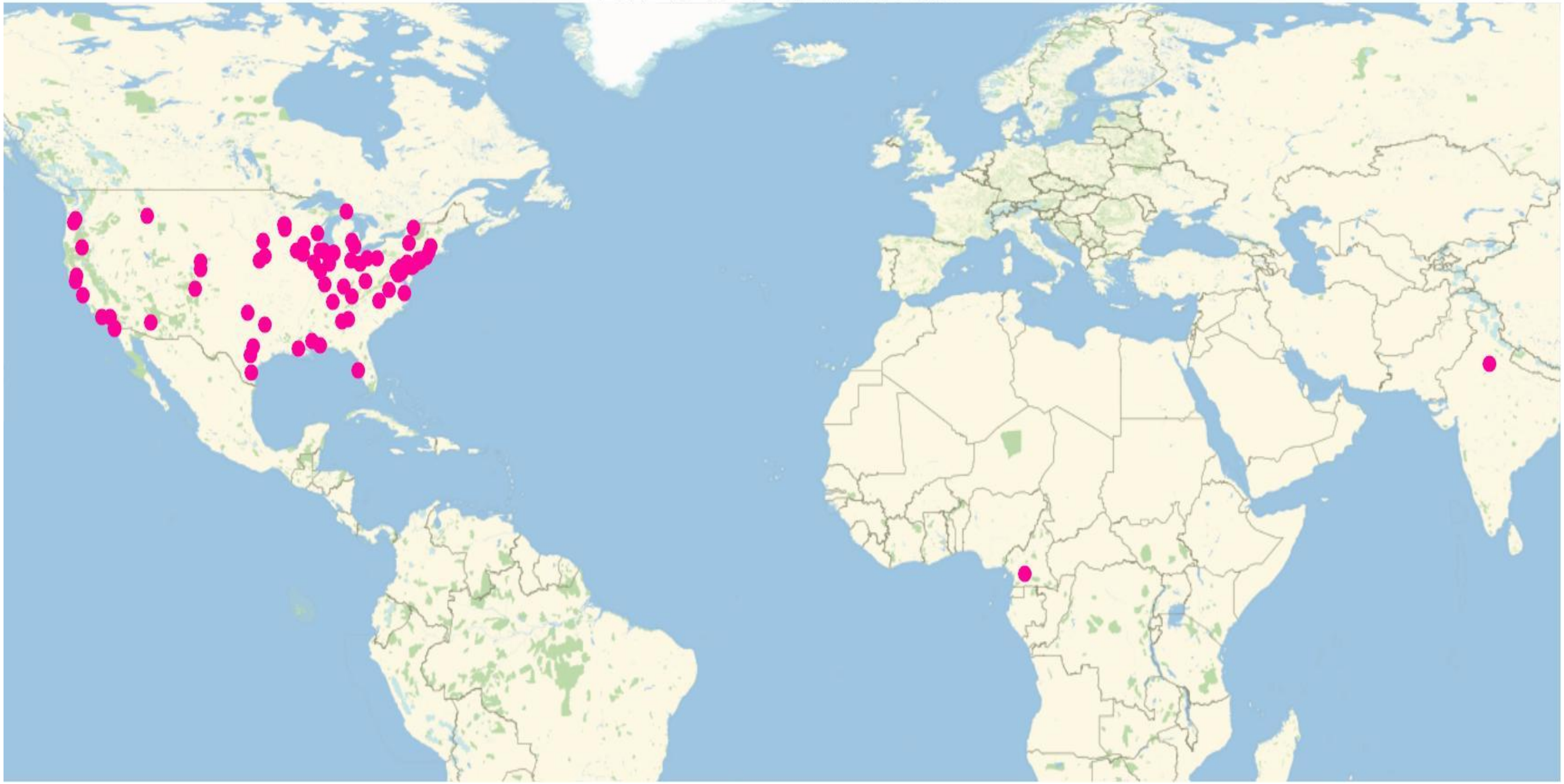

More questions/conversations?

Thank you for your engagement.

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