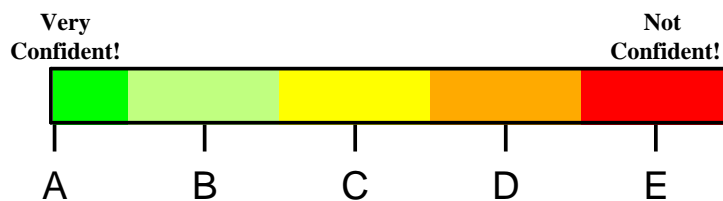


Chem 5181: Mass Spectrometry

Ingrid Ulbrich

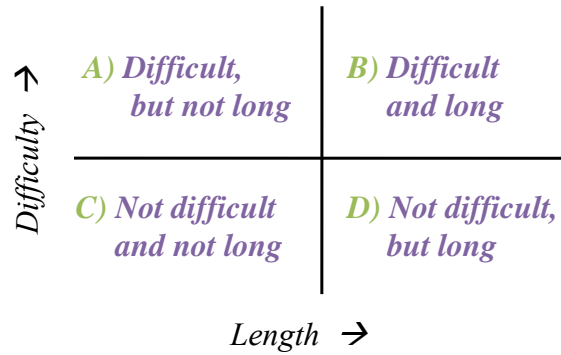
27 August 2009

How do you feel now
about that homework?



Confidence Scale

How long vs. hard was that homework?



Numerical Integration in Igor

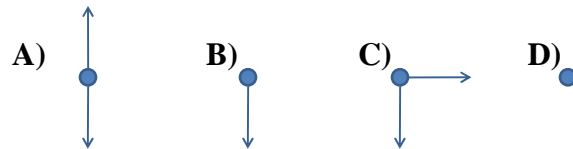
Tossing a ball in the air

or

What goes up must come down

Simple Case:
Toss a Ball *Straight Up* in the Air

When the ball is in the air, what is the force diagram for the ball?



E) None of These

Simple Case:
Toss a Ball *Straight Up* in the Air

- What will the trajectory of the ball look like?

x vs. t

y vs. t

x vs. y

Let's work to plot y vs. t

1. Make a wave of time in seconds.

➤ Let's start a function:

- Make/O/N=10 time_s // time in seconds
- time_s = x // for now 1s increments

Simple Case:

Toss a Ball *Straight Up* in the Air

Acceleration is...

- A) constant B) proportional to t C) proportional to t^2
D) none of these

Acceleration is equal to... **-g**

- Let's make a **CONSTANT** above the function
- Now we can make a wave for accel_m_s2

Simple Case: Toss a Ball *Straight Up* in the Air

Velocity is...

- A) constant B) proportional to t C) proportional to t²
 D) none of these

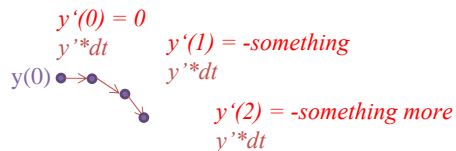
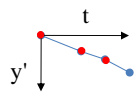
Velocity is related to *acceleration* by... $a = dv/dt$

$$dv = a*dt$$

Integrating Acceleration → Velocity

We'll use Euler's Method:

$$y(i) = y(i-1) + y'(i)*dt$$



∫ line = parabola

Since we already “know” how to calculate the answer...

- Let’s make a table to calculate (check) what we expect to get for velocity

Acceleration (m/s ²)	Time (s)	Velocity (m/s)
	0	
	1	
	2	
	3	

Since we already “know” how to calculate the answer...

- Let’s make a table to calculate (check) what we expect to get for velocity

Acceleration (m/s ²)	Time (s)	Velocity (m/s)
-9.8	0	
-9.8	1	
-9.8	2	
-9.8	3	

Need an initial condition!

Let’s just drop the ball. Then $v_0 = ?$

Since we already “know” how to calculate the answer...

- **Let’s make a table to calculate (check) what we expect to get for velocity**

Acceleration (m/s ²)	Time (s)	Velocity (m/s)
-9.8	0	0.0
-9.8	1	
-9.8	2	
-9.8	3	

Since we already “know” how to calculate the answer...

- **Let’s make a table to calculate (check) what we expect to get for velocity**

Acceleration (m/s ²)	Time (s)	Velocity (m/s)
-9.8	0	0.0
-9.8	1	- 9.8
-9.8	2	-19.6
-9.8	3	-28.4

How do we tell the computer how to do this calculation?

1. Use the *initial condition* to fill in the first element of the wave.
 2. For every row in the rest of the wave, calculate
$$v_i = v_{i-1} + a_i * dt$$
- In the function we can do step 1:
- Create a variable `v_0_m_s`
 - make `vel_m_s`
 - set zeroth point of `vel_m_s = v_0_m_s`

Writing the “for each row” part

Only happens when
entering the “for” loop
e.g. `index = 0`

Do stuff until this
isn't true anymore
e.g. `index < 100`

Only happens at the end
of the stuff inside the
“for” loop:
ready to do the next one
e.g. `index = index + 1`

`for(start counter; do it condition; update counter)`

stuff to do each time

usually depends on the counter

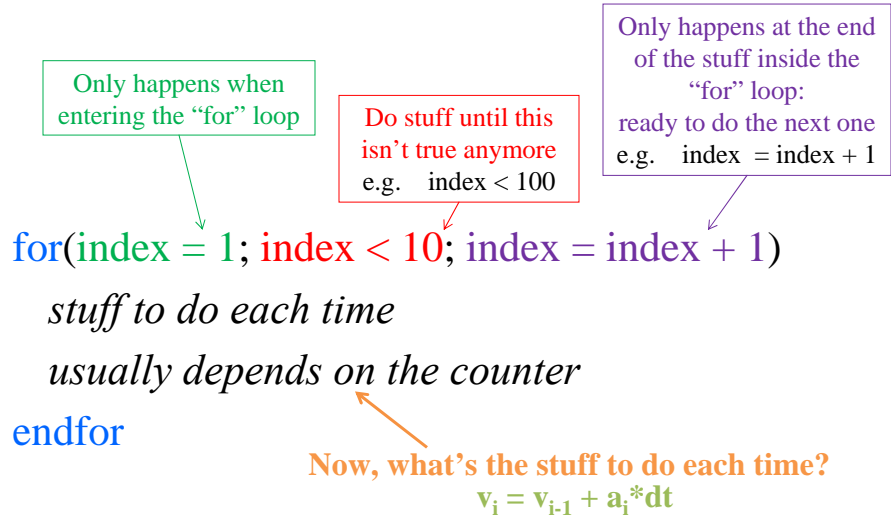
`endfor`

The “index” for our case

Igor Row Number	Acceleration (m/s ²)	Time (s)	Velocity (m/s)
0	-9.8	0	0.0
1	-9.8	1	- 9.8
2	-9.8	2	-19.6
3	-9.8	3	-28.4

- Row 0 was special, and we’ve already handled that
 - `Vel_m_s[0] = v_0_m_s`
 - So we want to start our integration with row 1
 - Make counter start at `index = 1`
- We want to operate on every row
 - Increase our counter by `index = index + 1`
- We want to keep going while we have rows
 - Stop Condition is `index < 10`

Writing the “for each row” part



A closer look at our equation

Vel_m_s *accel_m_s2*

$$\mathbf{v}_i = \mathbf{v}_{i-1} + \mathbf{a}_i * dt$$

can get dt from time_s

\mathbf{v} , \mathbf{a} , and t already exist in our function!

So how can we write the equation?

Now Run with Debugger

- Procedure → Enable Debugger
- In the new column at the left, click in a row in the function.
 - This will stop execution of the function and start the debugger.
- Above the top center box in the debugger, chose “Local and Global Variables”
- The yellow arrow in the function shows the next line to be executed.
 - Proceed 1 line at a time by pressing enter or using the yellow arrow button at the top of the debugger.
 - Proceed to next stop (or end) by pressing the green arrow button at the top of the debugger

Simple Case:
Toss a Ball *Straight Up* in the Air

Position is...

- A) constant B) proportional to t C) proportional to t²
D) none of these

Position is related to *velocity* by ... $v = ds/dt$

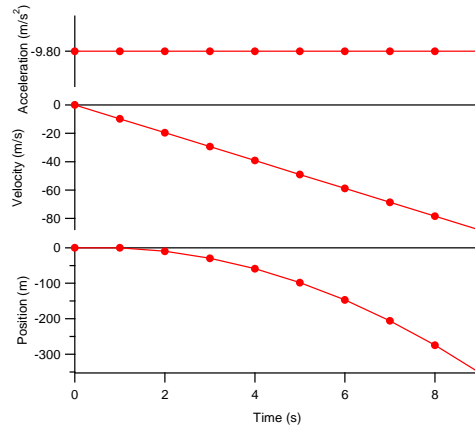
$$ds = v*dt$$

How can we implement the
position calculation?

- A. Position *must* be calculated in a **different function**.
- B. Position can be calculated in a *separate for* loop *before* calculating the velocity.
- C. Position can be calculated in a *separate for* loop *after* the loop for calculating velocity.
- D. Velocity and position can be calculated in the **same for** loop.

Let's make a plot!

- Make your axes like this
 - Spacing, alignment
 - Axis labels
 - Zero line for velocity, position
- Markers are nice, but not necessary



Next Steps

- Change v_0 and s_0 and see changes
- Generalize the function with input variables
- Assume that
 - $s_0 > 0$
 - the ground = 0
 - After the ball hits the ground it stays there for all remaining time

Ingrid's Office Hours for this Homework

Today: until 6pm

Friday: 10 am – 6 pm

Saturday: none

Sunday: 1-5 pm in the UMC near Domino's

Monday: 11 am – 6 pm

Charge Between Two Plates

