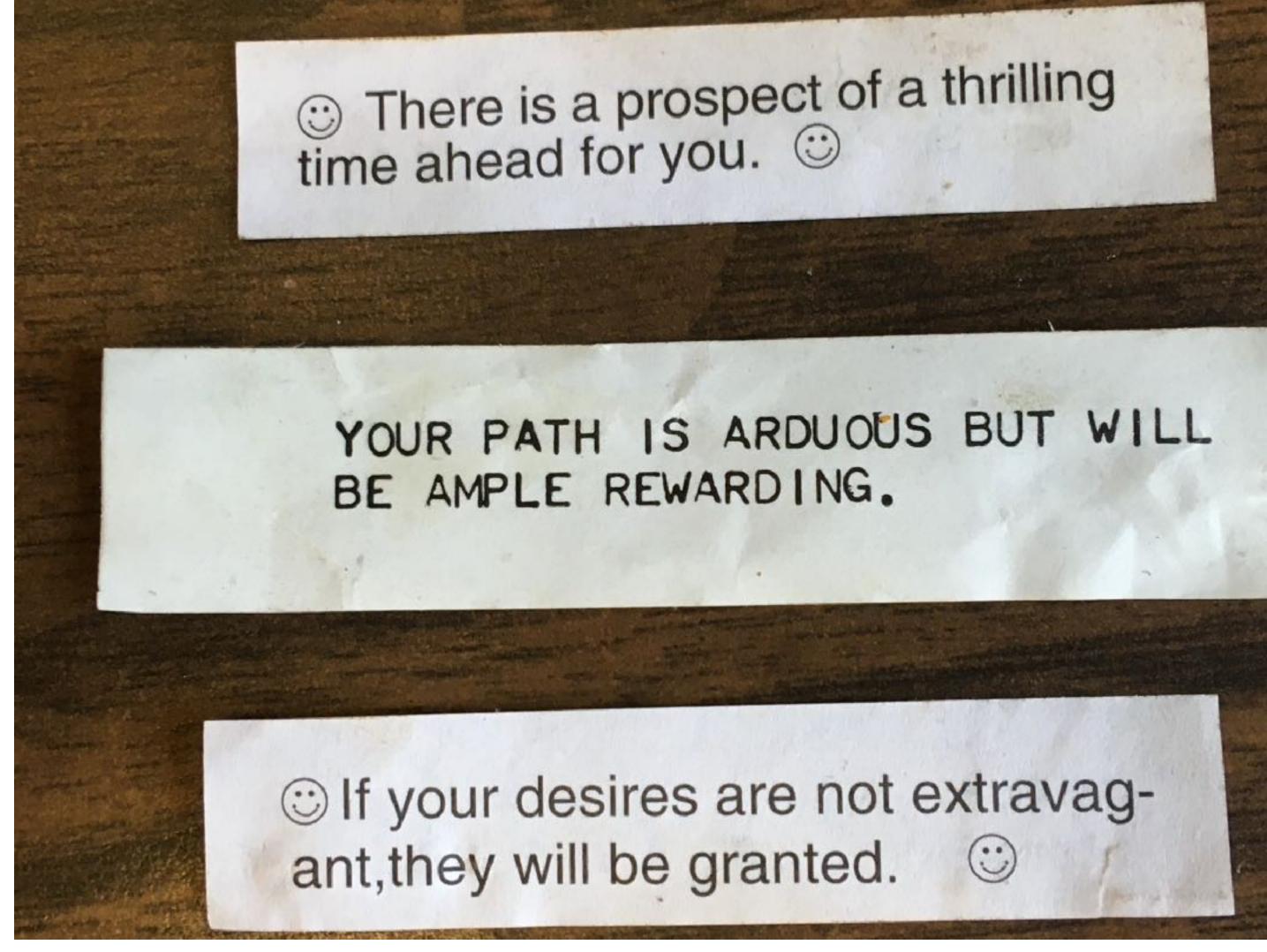
Phil Nelson, Univ of Pennsylvania

These slides will appear at www.physics.upenn.edu/~pcn



Scientific animation with Python

Story-telling with time

The best

The best questions are ones that you ask yourself.
The best images, still or animated, are ones you make for yourself.
Borrowing animations from Wikipedia only takes you so far!

The goals today are

- * Show what is possible and why you may want it.
- * Help you get started with one of a menu of Challenges.

What's the big deal?

Technically there's no big deal. A video is a bunch of still frames presented in succession at over 10/second (looks smoother if it's over 25/second).

But psychologically it's a big deal: We process stories as narrative, with plots.

We'll see how you can just get Python to spit out a lot of individual frames, then show them to you at a chosen rate.

But you'll also want to share your joy – in a presentation; in the supplement to your big article; on social media; etc. For this you need to stitch them together into a file in one of the usual formats, typically mp4 or m4a.

- You could make a video screenshot of Python playing your animation, e.g. with screenshot.app. Usually poor resolution and wrong speed.
- Or you can emit individual frames and postprocess with ffmpeg, QuickTime, iMovie, VLC, ImageJ, or another such free helper app.
- Today explore a third method: more convenient, once you get over the learning curve.

It's true that "play" can involve frustration. Your assistant is not necessarily your friend.

But your presentations will never be the same!

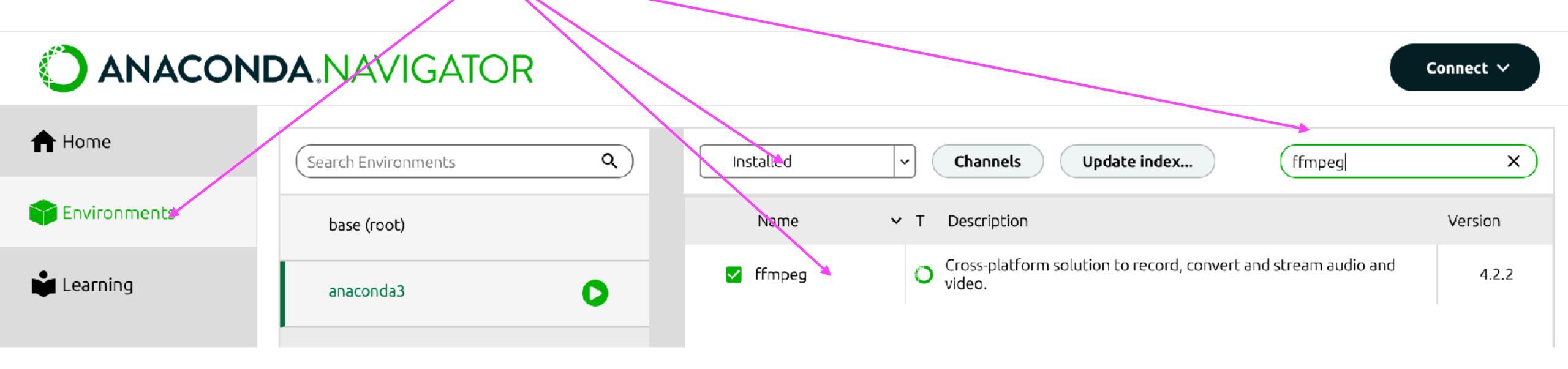


From Terminal app (macOS) or Anaconda Prompt app (Windows):

- \$ conda install ffmpeg
- \$ which ffmpeg
 /Users/pcn/anaconda3/bin/ffmpeg

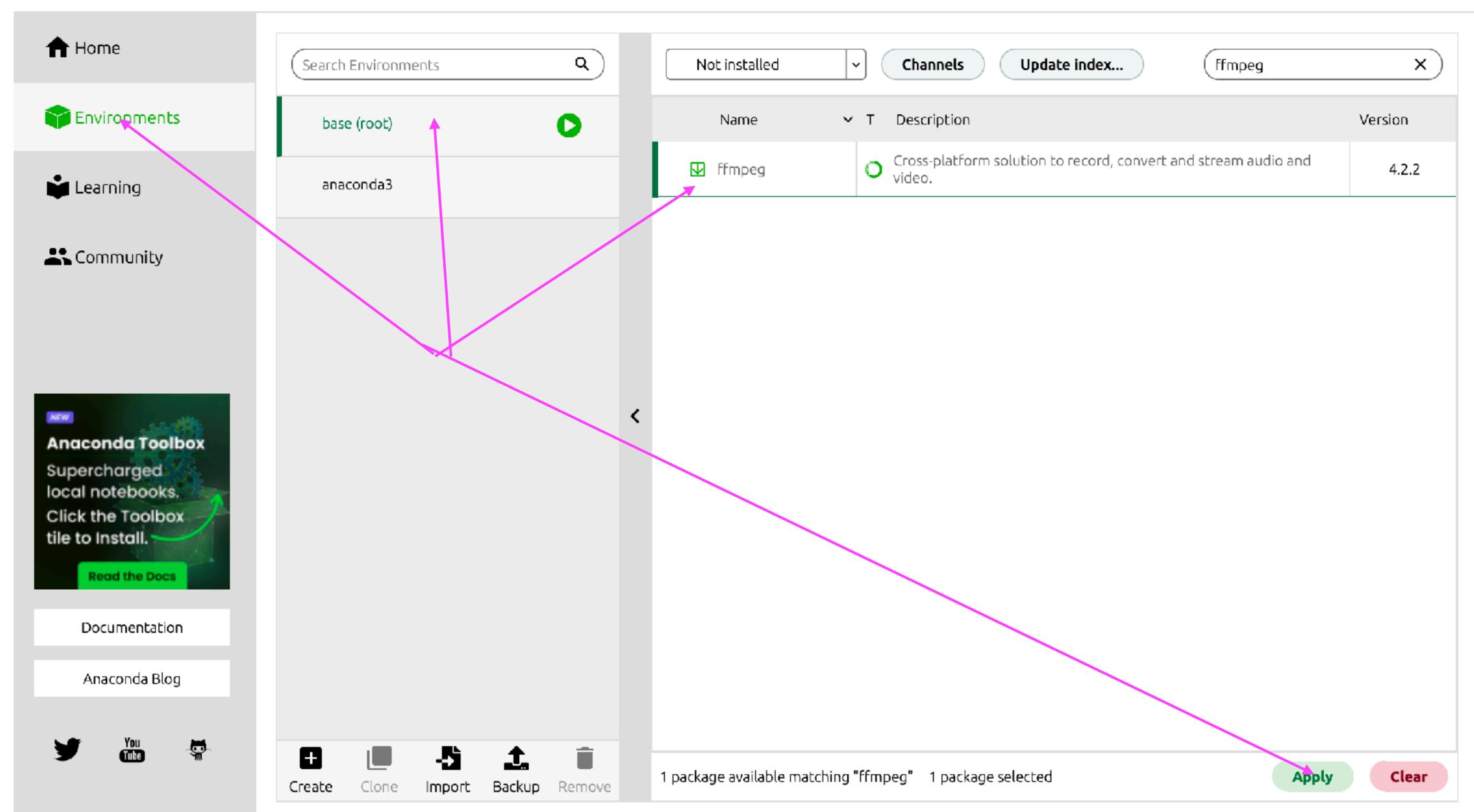
From inside Jupyter: %conda install ffmpeg

From Anaconda Navigator app:









Part 1: Beginning

When I was an undergrad, my lab had an ancient computer that was maintained only because it was the model on which Spacewar had been developed. Grad students would come in with huge bags of potato chips and spend the evening. Why was it so compelling? Well, something was *moving* on that screen. We are animals and we pay attention to moving things.

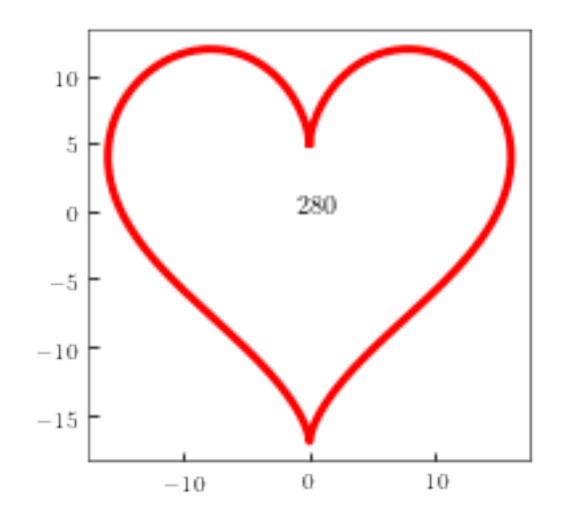
In your own presentations, you can make a traditional graph and say "here horizontal position represents time." But why not let *TIME* represent time? We process ideas as narratives; a process unfolds over time.

```
In [3]: import numpy as np; import matplotlib.pyplot as plt

# Generate plotting values
t = np.linspace(0, 2*np.pi, 200)
x = 16 * np.sin(t)**3
y = 13 * np.cos(t) - 5 * np.cos(2*t) - 2 * np.cos(3*t) - np.cos(4*t)

# Make the plot
plt.figure(figsize=(3,3))
plt.plot(x, y, 'r', linewidth=3)
plt.text(-1,0,'280')
```

Out[3]: Text(-1, 0, '280')



I'd like a more impactful valentine, one that grows and shrinks over time. Right away, I face a problem: My assistant, trying to please me, will rescale the axes in every frame so that the heart fills the frame! Instead of a fluctuating heart, I'll get fluctuating axes labels! There are various workarounds, but the general-purpose insight is that I want to make the axes *once*, then serially replace the contents always leaving the axes unchanged.

Pythonic matters

plt.figure() creates a "figure object," i.e an "object" in the class figure, and makes it the "current figure."

Objects can contain other objects. For graphing, we want our figure object to "own" an "axes object."

plt.axes() creates such an object in the current figure and makes it the "current axes."

An axes object can in turn contain, e.g. the lines that we usually think of as the axes, but also tick marks, labels, as well as data represented as symbols, curves, bars, etc.

plt.plot conveniently combines several operations:

- create a figure object if none exists and make it "current figure" (otherwise use the existing current figure).
- add an axes object to the current figure object if none exists and make it "current axes."
- add symbols and/or curves to that axes object to represent data.
- revise the limits and labels as needed to accommodate that plot and any others already present.

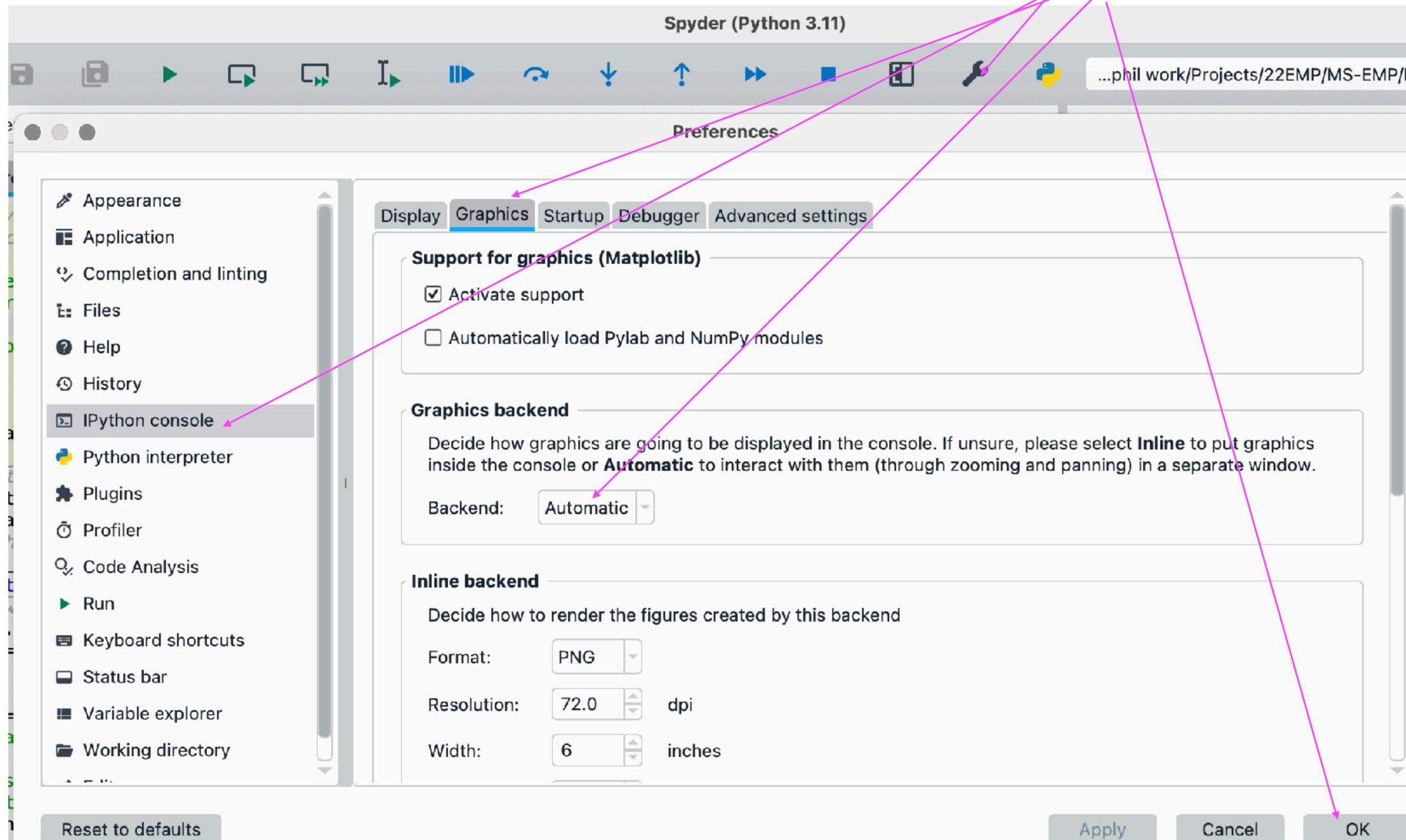
But those operations can be *unbundled* for greater control.

In particular, we may wish to attach names to certain subobjects, so that we can go back and modify them by calling their methods.

Thus, if my_ax is the name of an axes object then its method my_ax.plot() will draw a plot in that object, regardless of whether it is "current." It also returns a tuple containing the object(s) it created (lines, symbols, etc.); if we wish we can assign a name to it. Later, we can then use that handle to *change subobjects of the plot without completely redrawing it*.

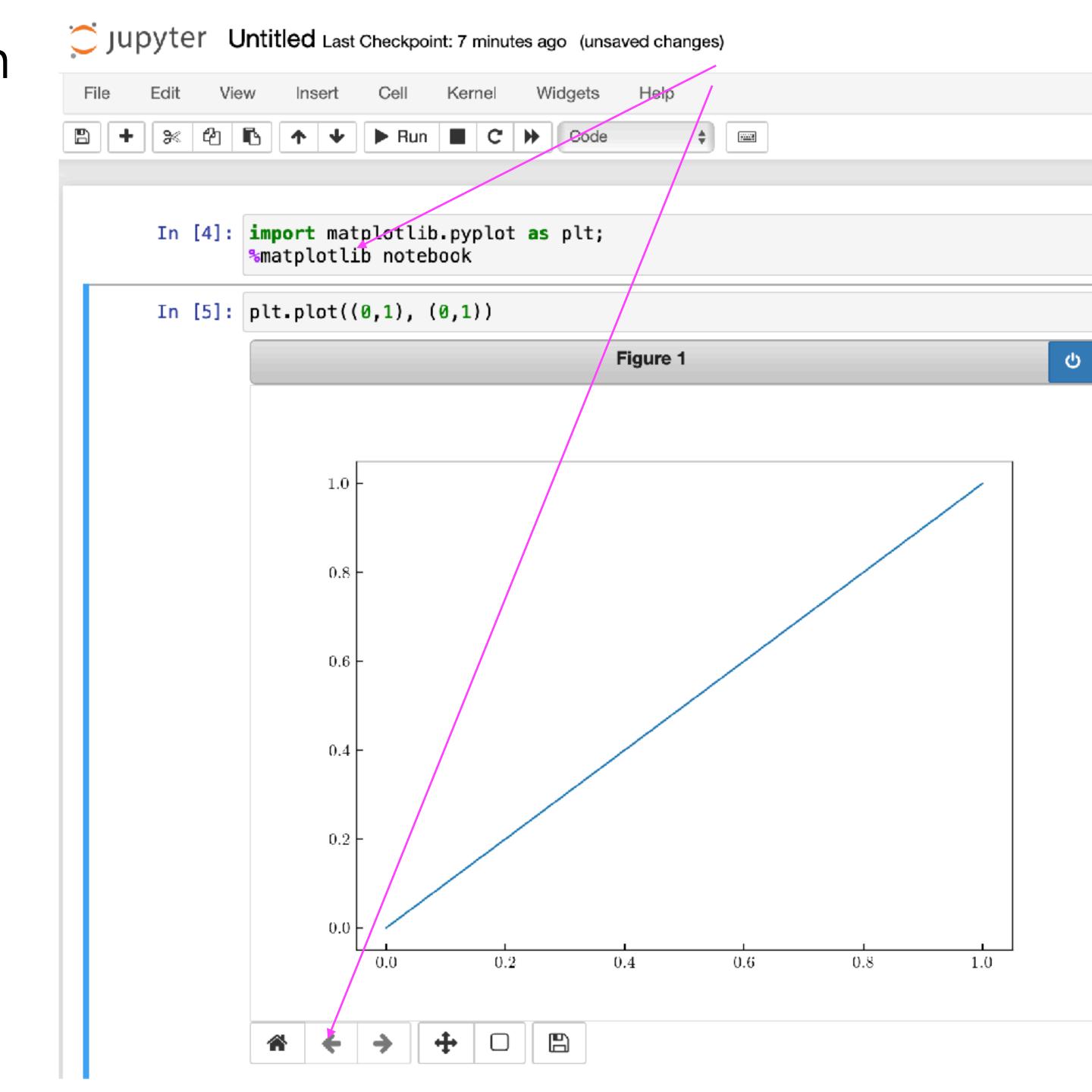
First set your environment to give "live plots." In Spyder, you only need to do this once:

Making live plots on your screen (Spyder)



Making live plots on your screen (Jupyter)

Do this every session:



Making live plots on your screen (Colab)

Do this every session:

```
!pip install ipympl
from google.colab import output
output.enable_custom_widget_manager()
%matplotlib widget
```

Extracting the files you write (Colab)

```
from google.colab import files
# bring output file to my (real) machine's Downloads folder:
files.download('filename.mp4')
```

```
[ https://stackoverflow.com/questions/62275854/is-there-any-way-to-interact-with-matplotlib-figures-in-google-collaboratory/70482960#70482960 ] [ https://colab.research.google.com/notebooks/io.ipynb#scrollTo=vz-jH8T_Uk2c ]
```

heartThrob.py:

In Python, a function has access to variables defined in the surrounding code.

Sticklers may prefer to transmit them via the "fargs" keyword in FuncAnimation.

A "return" statement here is optional.

Assigns a name to the first (and only) line object in the plot. That comma is crucial to unpack the returned tuple.

```
import numpy as np; import matplotlib.pyplot as plt; plt.close("all")
from matplotlib import animation
#%% set up: get_step draws a frame and is called by FuncAnimation below:
def get_step(n):
    scale = np.abs(np.sin(2*np.pi*(n/30))) # this changes for each frame
   # heart and my_line are defined outside the function but available inside it:
   my_line.set_data(scale*heart[0], scale*heart[1])
#%% now begin the main code: set generic graph values:
t = np.linspace(0, 2*np.pi, 200)
heart = [16 * np.sin(t)**3, 13 * np.cos(t) - 5 * np.cos(2*t) - 2 * np.cos(3*t) - np.cos(4*t)]
my_fig = plt.figure()
my_ax = plt_axes(xlim=(-20,20), ylim=(-20,20)) #exactly the same in every frame
"""create an empty curve, which will be replaced for every frame, and assign it
a name so that we can manipulate it. """
(my_line, ) = my_ax_plot([], [], lw=3, color='red')
"""Now make the animation:
Tell FuncAnimation which figure window, what frame-drawing function to use, how
many frames. blit is optional:
my_movie = animation.FuncAnimation(my_fig, get_step, frames=60, blit=True)
```

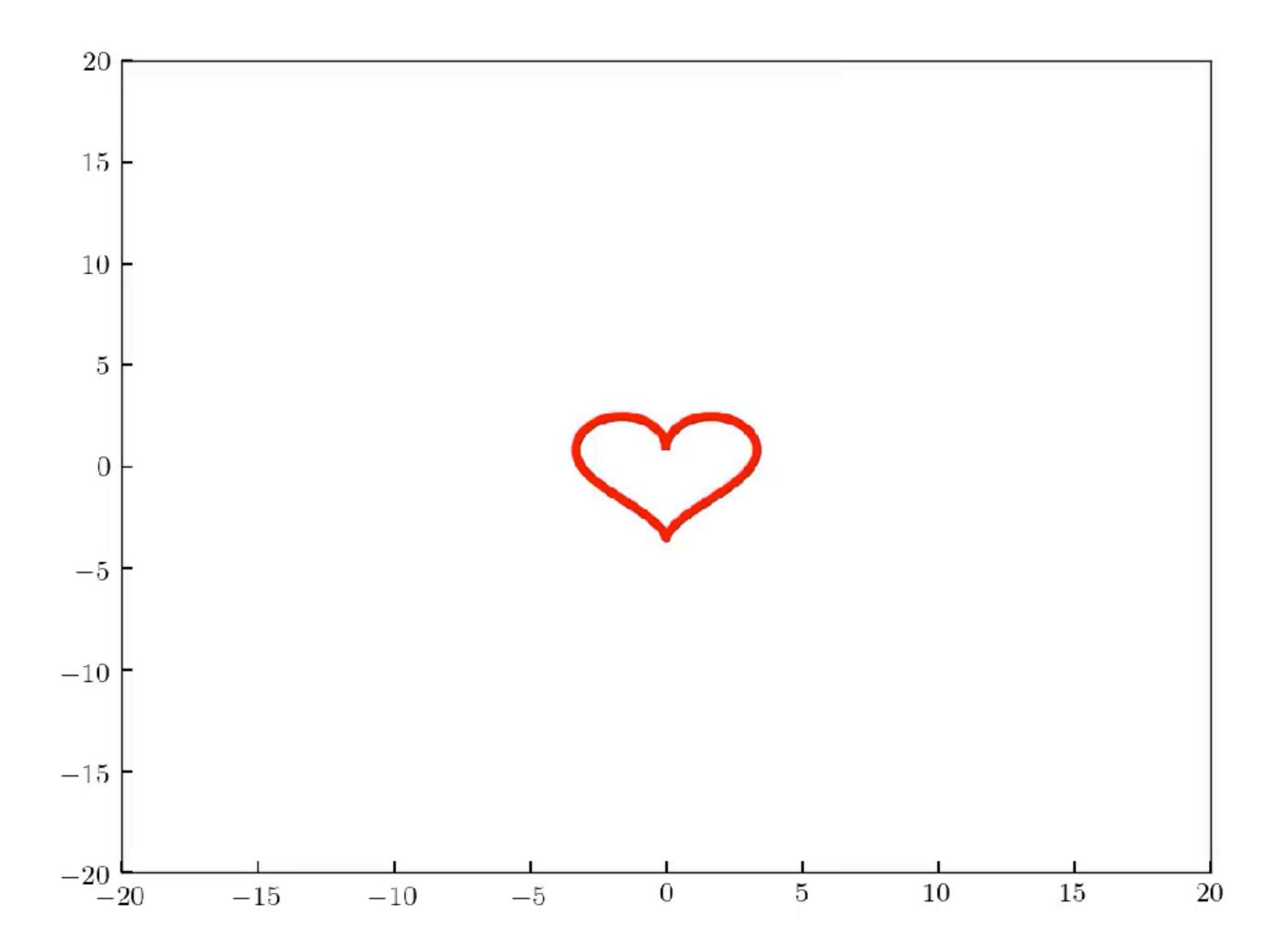
You can now just do a video screen shot of the animation while Python is displaying it. Or, if you have installed ffmpeg properly, add

my_movie.save('filename.mpg')
to your code.

(ffmpeg is automatically available in Colab.)

There are useful optional arguments available for the save method, including fps ("frames per second") and dpi ("dots per inch").

The resulting mpg, m4a, etc file is then suitable for placing in a presentation (as I have done here), posting to the Web, etc.



Challenges to think about

Challenge: Draw a fixed Lissajous figure, then an animated dot that traces it. Then do something cool on you own initiative.

[This is the parametric curve $x = P \sin(At)$, $y = Q \sin(Bt)$.]

Challenge: Draw a fixed epicycloid or hypocycloid figure, then an animated dot that traces it. Then do something cool on you own initiative.

[This is the parametric curve $x = \sin t + P \sin(At)$, $y = \cos t + P \cos(At)$.]

More challenges

Challenge: Draw a progressively evolving planetary orbit with perihelion precession. That is, the curve should be the open curve

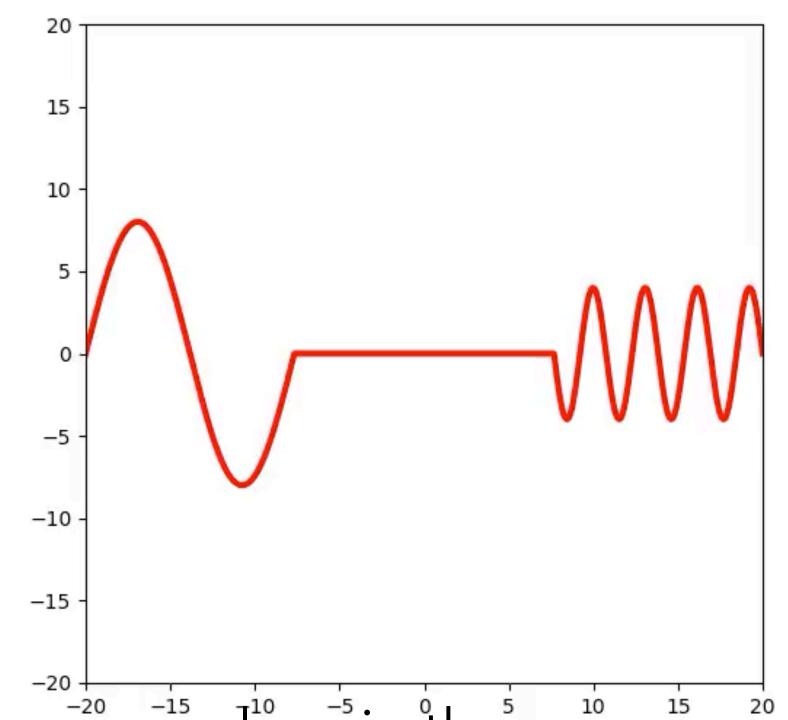
$$r(\theta) = (1 + b\cos(q\theta))^{-1}$$

where q is close to, but not exactly equal to, 1.

Moreover, trace out the curve at variable speed determined by angular momentum conservation: $d\theta/dt = 1/r(\theta)^2$.

Notes: Things have been nondimensionalized by convenient units of time and space. The value of b controls the eccentricity (b=0 means circular orbit, so don't use that value).

Traveling waves (sound in air or light in vacuum):



Challenge: make a delta function out of cosine waves. Let each one evolve via the Schrodinger equation, and thus see how that delta wavepacket spreads. Actually, forget about the SE: All you need to know is that each component wave has frequency related to its wavenumber via $\omega = k^2$. And your starting superposition is a bunch of cosines all with equal weight (the Fourier transform of a delta function). [Thus the real part of the wavefunction is $f(x,t) = \sum \cos(kx + k^2t)$ where k ranges over, say, -50, -49.8, -49.6,..., +50.]

Time evolution of a distribution

Molecular diffusion involves the spread of a distribution. It's instructive to look at the randomness in a single instance. But instead of a single histogram at final time, why not make a video of the time development of the histogram?

```
def get_step(n):
    for i in range(Nbins):
        my_bars[i].set_height(binpops[i,n])
```

To animate bar plot, in each frame reset the array of bar heights.

Random walkers in potential trap

The distribution spreads at first, then stops spreading. It also migrates, slowly, 250 eventually becoming centered on the bottom of the potential energy well (x=50).

A movie object returned by FuncAnimation contains a "save" method.

This one line renders the animation and writes it to a file for use elsewhere:

my movie.save('harmonicRW.mp4',

200 150 population 5020 60 80 100

Brownian in a trap: Details

How to animate bar plot

```
myfig = plt.figure() # set up one invariant axes for all frames
movie_ax = plt_axes(xlim=(-1,Nbins+1), ylim=(0,Nwalk/2)) # must stay constant over many frames
binpops = np.zeros((Nbins, Nstep)) #history of histogram
half = Nwalk//2
binpops[3*Nbins//4,0] = half
binpops [-1+3*Nbins//4,0] = Nwalk - half
my_bars = movie_ax.bar(range(Nbins), binpops[:,0]) # first frame
#%%
for time in range(1,Nstep):
    temp = np.zeros(Nbins)
    temp[1] = binpops[0, time-1] #handle left edge separately: all bounce
    temp[-2] = binpops[-1, time-1] #handle right edge separately
    for xbar in range(1, Nbins-1): # exclude ends which were handled separately
        Pplus = (1 - (xbar - Nbins//2)/400)/2
        m = brn(binpops[xbar,time-1], Pplus) # partition walkers
        temp[xbar+1] += m
        temp[xbar-1] += binpops[xbar,time-1] - m
    binpops[:,time] = temp
    if temp.sum() != Nwalk: print("oops", time, binpops.sum()) #should never happen but check
#%%
def get step(n):
    for i in range(Nbins):
```

my_bars[i].set_height(binpops[i,n])

Another challenge

Challenge: simulate Ehrenfest's Fleas, and display the results as an animated bar chart. Then do something cool on you own initiative.

For example: Two dogs. 300 fleas. Initially all fleas are on dog #0. On each time step one randomly-chosen flea will switch dogs.

Second visualization: The Swarm

This time, compute the actual trajectories of just 20 walkers. Release the walkers at a variety of initial positions, say, evenly spaced at $\bar{x} = 2, 7, 12, ... 97$. Where do they end up?

```
myfig = plt.figure(figsize=(6,1)) # set up one invariant axes for all frames
movie_ax = plt.axes(xlim=(-1,Nbins+1)) # must stay constant over many frames
my_gnats = movie_ax.scatter(trajects[:,0], np.zeros(Nwalk))

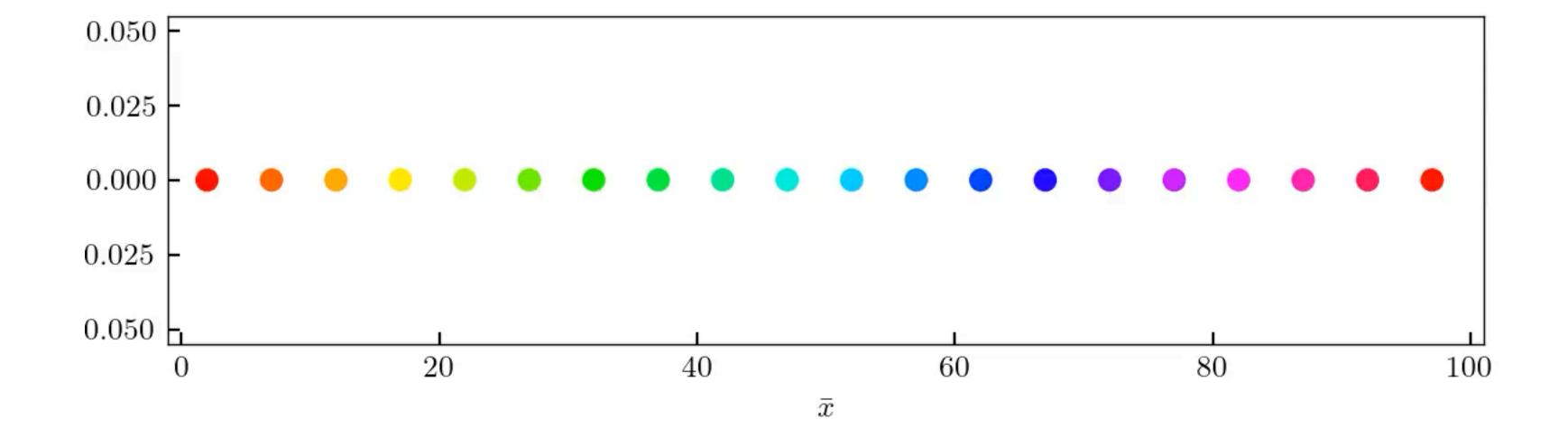
<< blah blah, create trajects[which walker, which time] >>

def get_step(n):
    my_gnats.set_offsets(np.vstack((trajects[:,n],np.zeros(Nwalk))).T)
```

To animate scatterplot, in each frame reset the xy values by supplying an array with 20 rows and two columns.

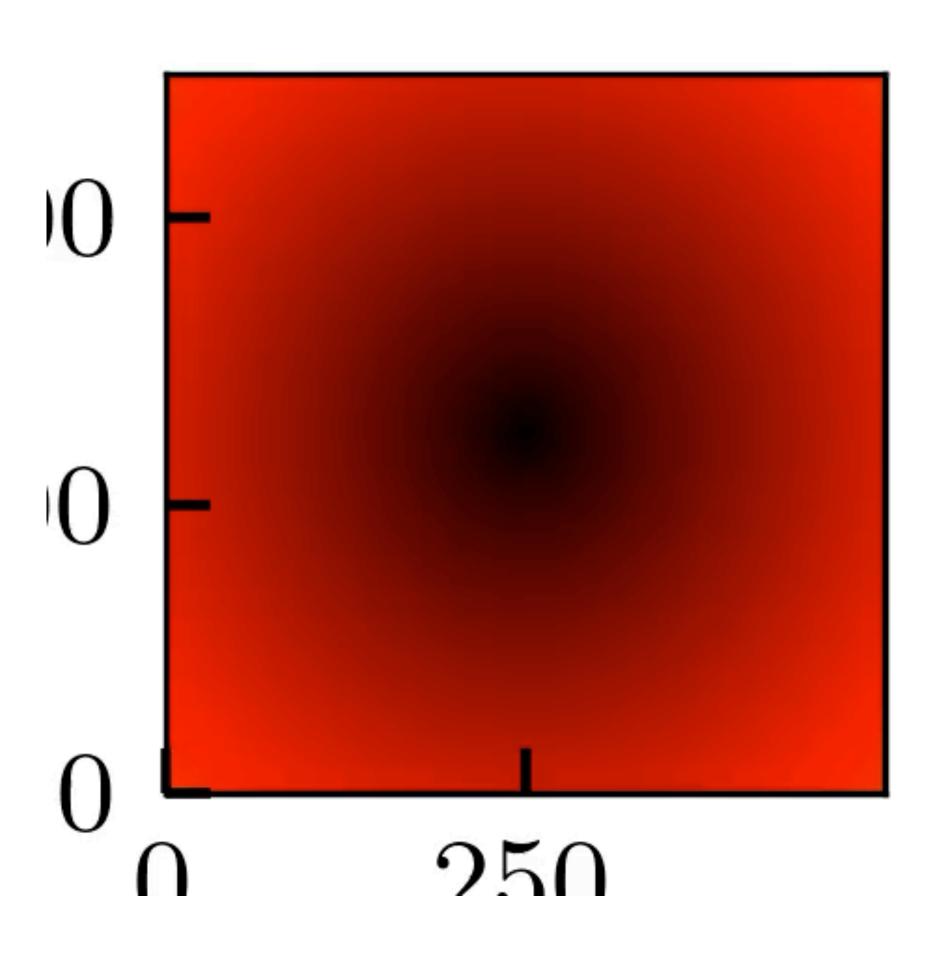
Finally, let's distinguish each walker by giving each its own color. There are various ways to do this. [Hint: Check the documentation for scatter for its keyword argument color.]

The walkers never stop getting transiently pushed out to large excursions.



Raster=bitmap=heatmap Animation

$$x^2 + \frac{y^2}{1.1 + \sin t}$$



Animating heat maps

```
fig, ax = plt.subplots(1, figsize={3.6,
image = ax.imshow(<<first frame>>>.T) # to be changed each frame
mobilepoint, = ax.plot([],[],'g*', ms=3) # to be changed each frame
mytext = ax.text(6,4,'variable label') # to be changed each frame
plt.xlabel(r'$x$\ [a.u.]')
                                  # fixed stuff
                          # fixed stuff
ax.text(6, 2.6, 'fixed label')
def animate(k): # make video frame k by changing what needs changing
   image.set_array(<<frame k>> T)
   mobilepoint.set data([position(k)], [0.])
   return image, mobilepoint, mytext # return changed objects
```

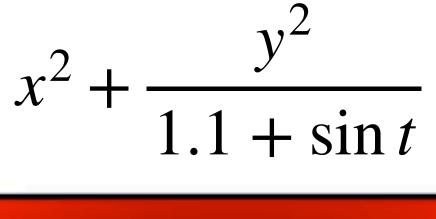
Challenge

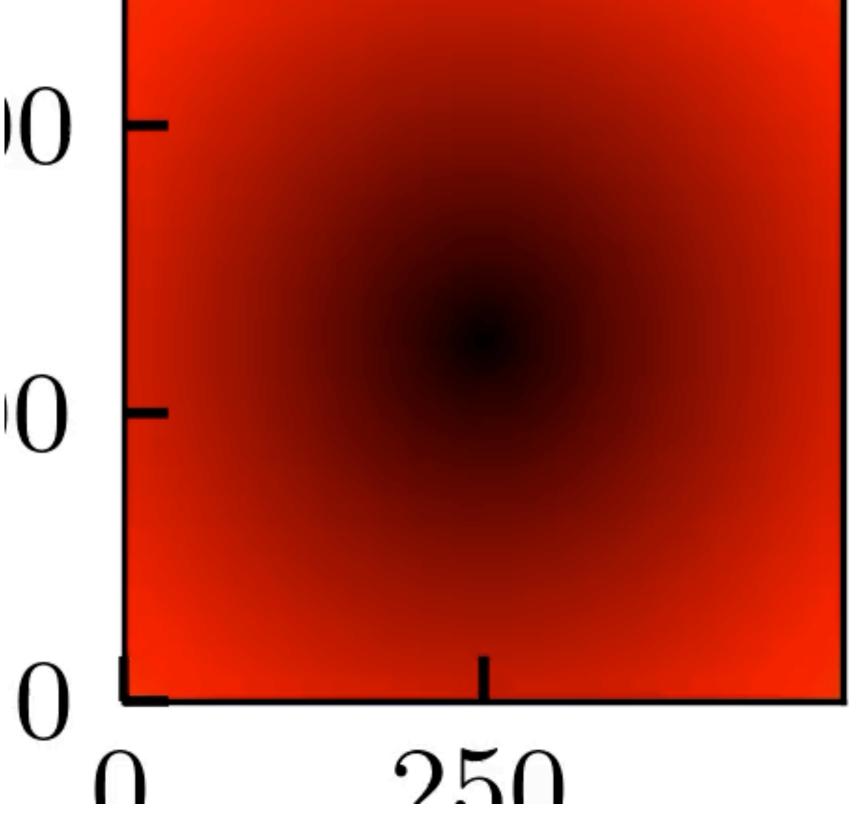
Challenge: Instead, show 2D diffusion from a point (or something more interesting) in such a representation: $c(t, \vec{x}) = t^{-1} \exp(-||\vec{x}||^2/t)$

Challenge: Instead, show the real part of a p orbital in the xy plane:

Re
$$\Psi(r, \varphi, t) = re^{-r}\cos(\varphi - t)$$

Challenge: The same, but this time as a surface plot.





Useful shortcut

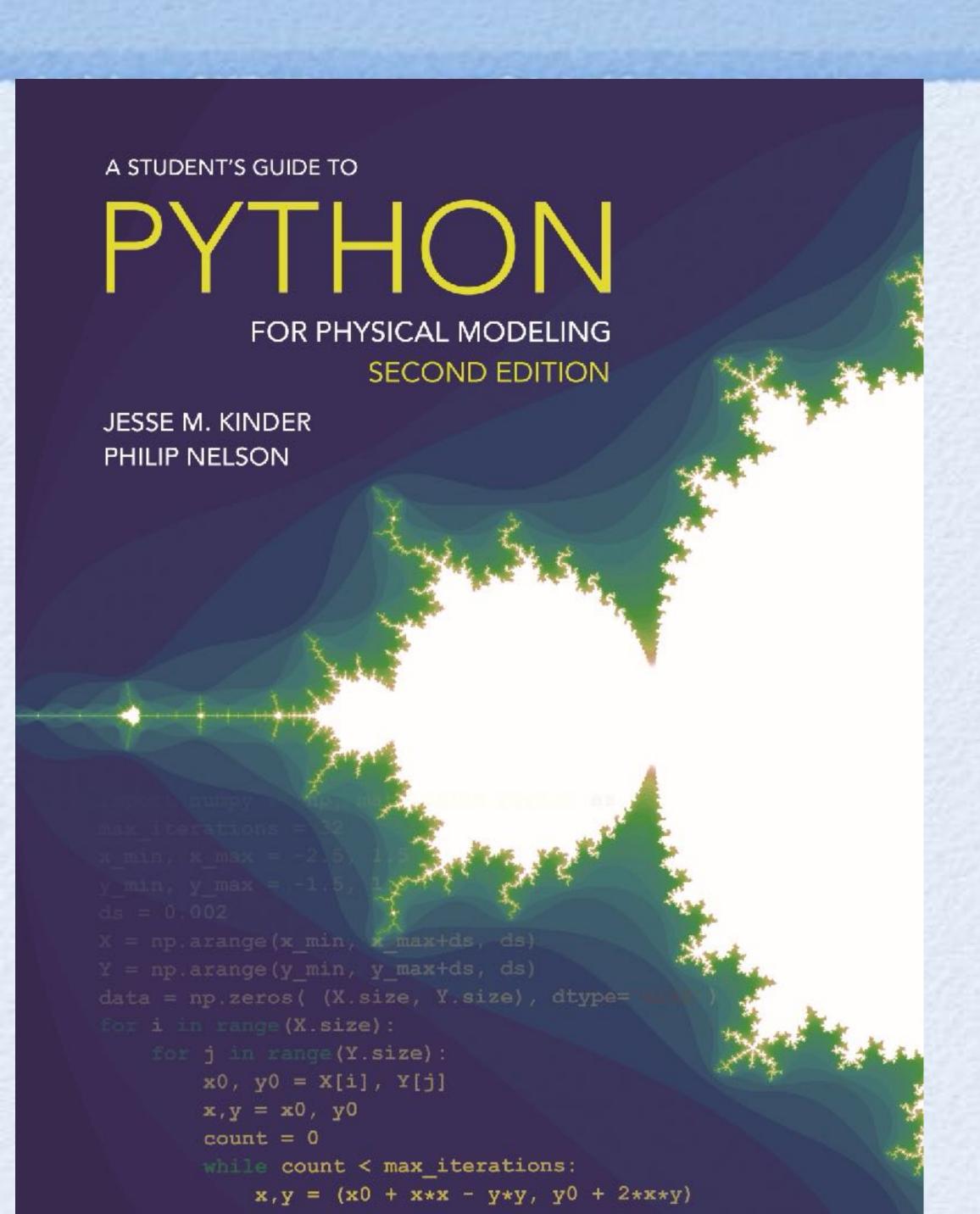
```
t = np.linspace(0, 5*np.pi, 101) # define parameter for parametric plot
ax.plot3D(t * np.cos(t), t * np.sin(t), t)
                                                           # generate 3D plot
# onward to animation
"""Easy matplotlib animation.
https://github.com/jwkvam/celluloid/blob/master/celluloid.py :"""
from celluloid import Camera
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')# create 3D plotting object attached to figure
ax.set_aspect('equal')
                                           # distortion? no thanks
camera = Camera(fig)
for thist in t:
   ax.plot3D(t * np.cos(t), t * np.sin(t), t, 'b')
                                                      # same in every fram
   ax.plot3D([thist * np.cos(thist)], [thist * np.sin(thist)], [thist], 'or')
   camera.snap()
animation = camera.animate(interval=100, blit=True)
```

The best

The best questions are ones that you ask yourself.

The best images, still or animated, are ones you make for yourself.

Go ahead.



<-- Princeton Univ Press, August 2021

Pine, D J. Introduction to Python for science and engineering. CRC Press 2019.

J W-B Lin, H Aizenman. E M Cartas Espinel, K Gunnerson, and J Liu, *Introduction to Python programming for scientists and engineers*. Cambridge Univ. Press 2022.

C Hill, Learning scientific programming with Python. Cambridge Univ. Press 2020.

THE CHALLENGES:

- Draw a fixed Lissajous figure, then an animated dot that traces it.
- Draw a fixed epicycloid or hypocycloid figure, then an animated dot that traces it.
- Draw a progressively evolving planetary orbit with perihelion precession.
- Make a delta function out of cosine waves. Let each one evolve via the Schrodinger equation, and thus see how that delta wavepacket spreads.
- Simulate Ehrenfest's Fleas, and display the results as an animated bar chart.
- Show 2D diffusion from a point as an animated heatmap.
- Show the real part of a p orbital in the xy plane as an animated heatmap. Or show the real part of a p orbital in the xy plane as an animated surface plot.

Part 2: Vistas

Some more use cases from my own research and teaching may give you ideas of your own.

- More stories about Brownian motion
- Story about adaptation in chemotaxis
- Stories about 3D objects in space
- Ray tracing for that meme-worthiness
- Electromagnetic radiation by accelerating charge.

Exporting animation by writing many still images

Here is a method that makes no use of matplotlib.animation:

```
nmesh = 500 # number of mesh points
tmin = -np.pi # start
tmax = np.pi # end
dt = 0.15 #
def x(i): # converts index to physical distance
    return 2.*(i/nmesh) - 1.0
def y(j): return 2**(j/nmesh) - 1.0
values = np.zeros((nmesh,nmesh)) # allocate
nframe = 0
for t in np.arange(tmin,tmax,dt):
    nframe += 1
    for i in range(nmesh):
        for j in range(nmesh):
            values[i,j] = np.sqrt(x(i)**2 + y(j)**2/(np.sin(t)+1.1))
    plt.imshow(values.T, cmap='hot', interpolation='nearest', origin='lower')
    plt.text(20, 50, 't='+format(t,'.2f'))
    plt.savefig('rasterMovie'+format(nframe,'05d')+'.png'); plt.close('all')
```

Then use an external helper app to postprocess the resulting image files. For example, Anaconda users can install FFmpeg via the Anaconda Navigator app, or by

\$ conda install ffmpeg (Windows: Can issue this command in Anaconda Prompt app.) (Mac: Use the Terminal app.)
Then use it:

\$ ffmpeg -i rasterMovie%05d.png -pix_fmt yuv420p rasterMovie.mp4

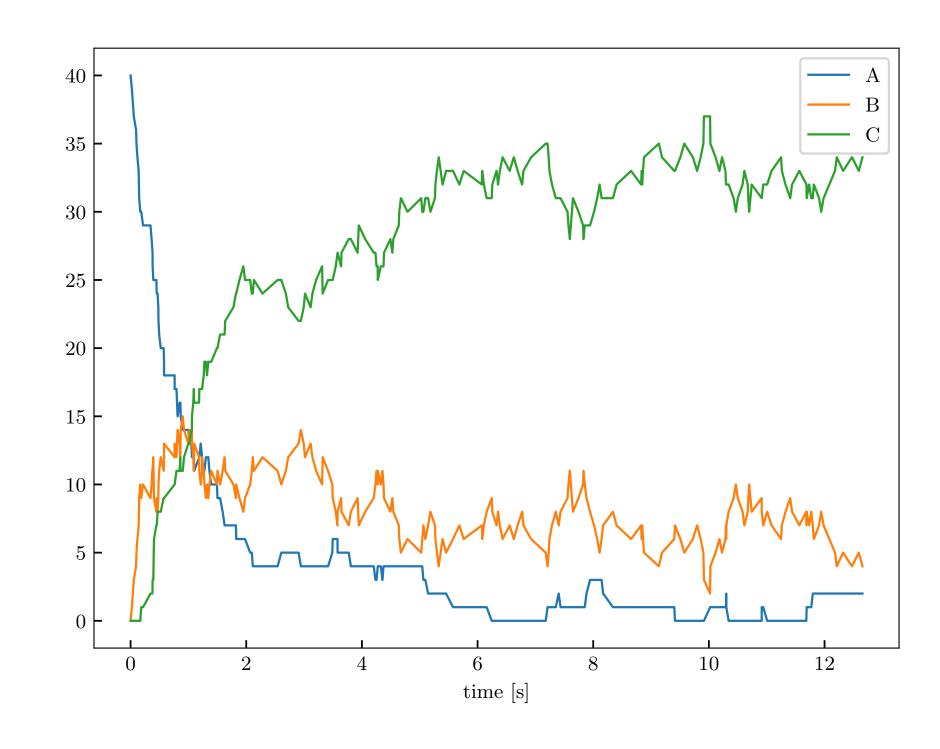
In case of error, may need (see https://stackoverflow.com/questions/20847674/ffmpeg-libx264-height-not-divisible-by-2)
 \$ ffmpeg -i rasterMovie%05d.png -pix_fmt yuv420p -vf "pad=ceil(iw/2)*2:ceil(ih/2)*2" rasterMovie.mp4

Exporting animation by linking FFmpeg to Python.

```
from matplotlib.animation import FuncAnimation
nmesh = 500 # number of mesh points
tmin = -np.pi # start
tmax = np.pi # end
dt = 0.15 #
all_times = np.arange(tmin, tmax, dt)
total_number_of_frames = len(all_times)
def x(i): # converts index to physical distance
    return 2.*(i/nmesh) - 1.
def y(j): return 2**(j/nmesh) - 1*
values = np.zeros((total_number_of_frames, nmesh, nmesh)) # allocate
nframe = -1
for t in all_times:
    nframe += 1
    for i in range(nmesh):
        for j in range(nmesh):
            values[nframe,i,j] = np.sqrt(x(i)**2 + y(j)**2/(np.sin(t)+1.1))
theTop = values.max(); theBot = values.min()
def animate(frame):
                           111111
    Animation function.
    global values, image # Not strictly neccessary
    image.set_array(values[frame].T)
    return image # return whatever you changed
animation = FuncAnimation(fig, animate, np.arange(total_number_of_frames),
    interval=1000 / 25)
# set the DPI to the actual number of pixels you're plotting to avoid interpola
animation.save("rasterMovie2.mp4", dpi=nmesh)
```

Boring kinetics

```
"""Description: demoThreestates.py Gillespie simulation of A<-->B<-->C model"""
import numpy as np; import matplotlib.pyplot as plt; plt.close('all')
from numpy.random import random as rng
"""Three states defining the cols of stoichiometry matrix:
     0 = A; 1 = B; 2 = C
Four reactions, all first-order, defining the four rows of stoichometry matrix:
     0 = A-->B; 1 = B-->A; 2 = B-->C; 3 = C-->B
stoich = np.array([[-1,1,0], [1,-1,0], [0,-1,1], [0,1,-1]]) # each row sums to 0
# rate constants:
ks = np.array([[1,0,0], [0,0.2,0], [0,1,0], [0,0,0.2]]) # only one entry in each row nonzero
Mtot = 40 # total number of molecs is constant
Ntrans = 250 # number of steps to simulate
pops = np.zeros((Ntrans+1, 3)) # allocate for populations in states A, B, C
pops[0, 0] = Mtot # initialize
ts = np.zeros(Ntrans+1) # allocate
rxnchooser = rng(Ntrans)
timechooser = rng(Ntrans)
for j in range(Ntrans):
    propens = np.sum(pops[j,:]*ks, axis=1) # propensities for each rxn
    norm = propens.sum() # prob/time for anything to occur
    breakpoints = np.cumsum(propens/norm)
    which event = np.searchsorted(breakpoints, rxnchooser[j])
    pops[j+1] = pops[j] + stoich[which event,:]
    ts[j+1] = ts[j] - np.log(timechooser[j])/norm
plt.figure(figsize=(3,3))
plt.plot(ts, pops)
plt.legend(('A','B','C'))
plt.xlabel('time [s]')
```

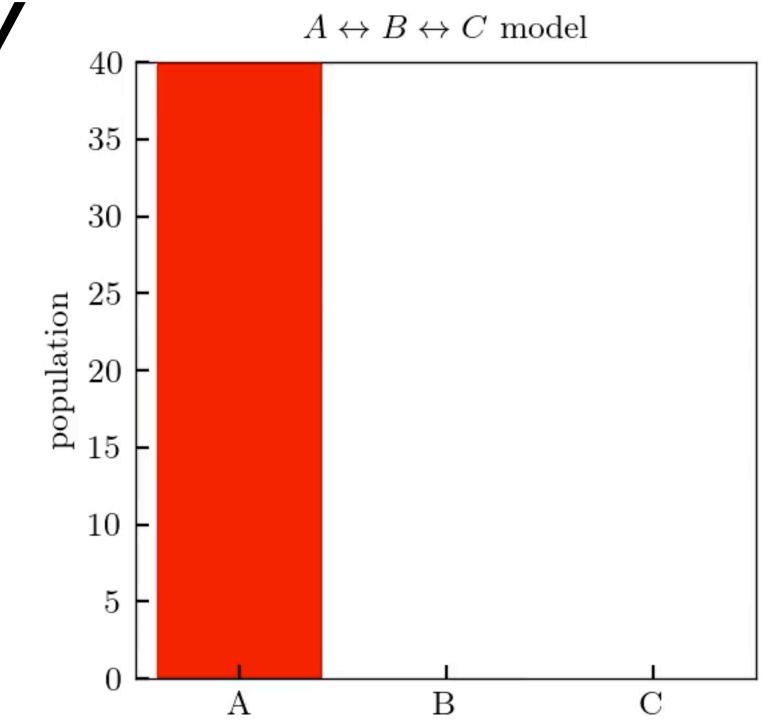


Kinetics as a thrilling story

Upgrade it to make a dancing bar-chart. To get started, initialize with

```
my_bars = movie_ax.bar(np.arange(0,3), np.zeros(3))
Then, in the animation function, modify the bars on each frame
using
```

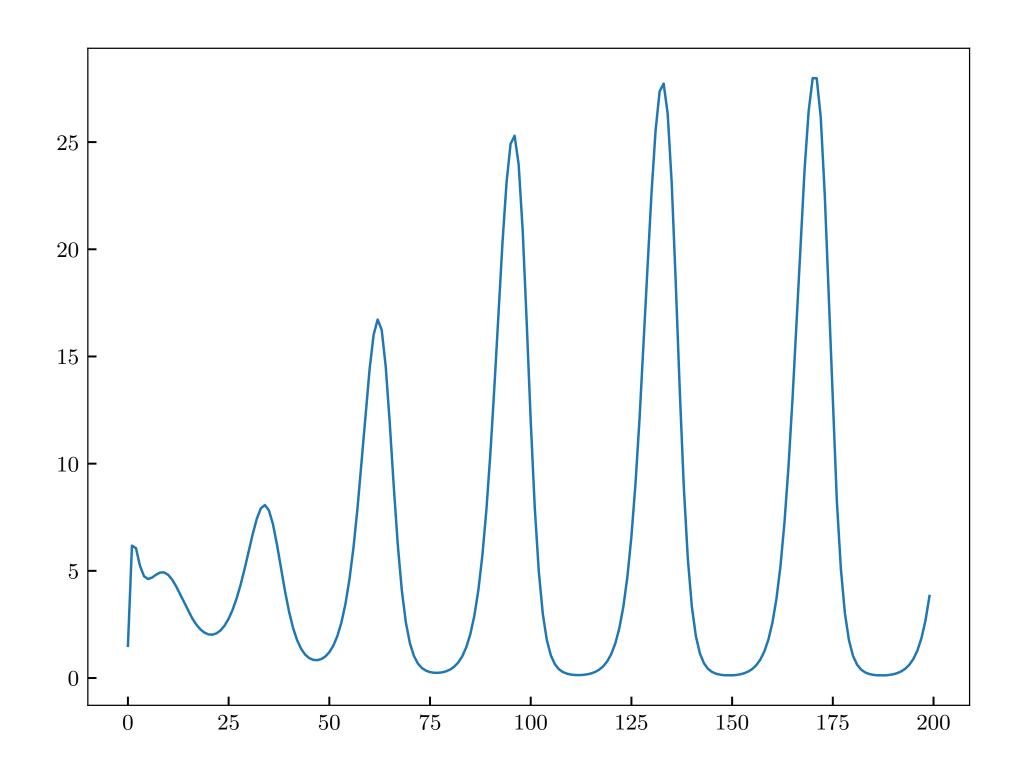
```
for i in range(3):
    my_bars[i].set_height(h[i,n])
where h is the result from your simulation.
```



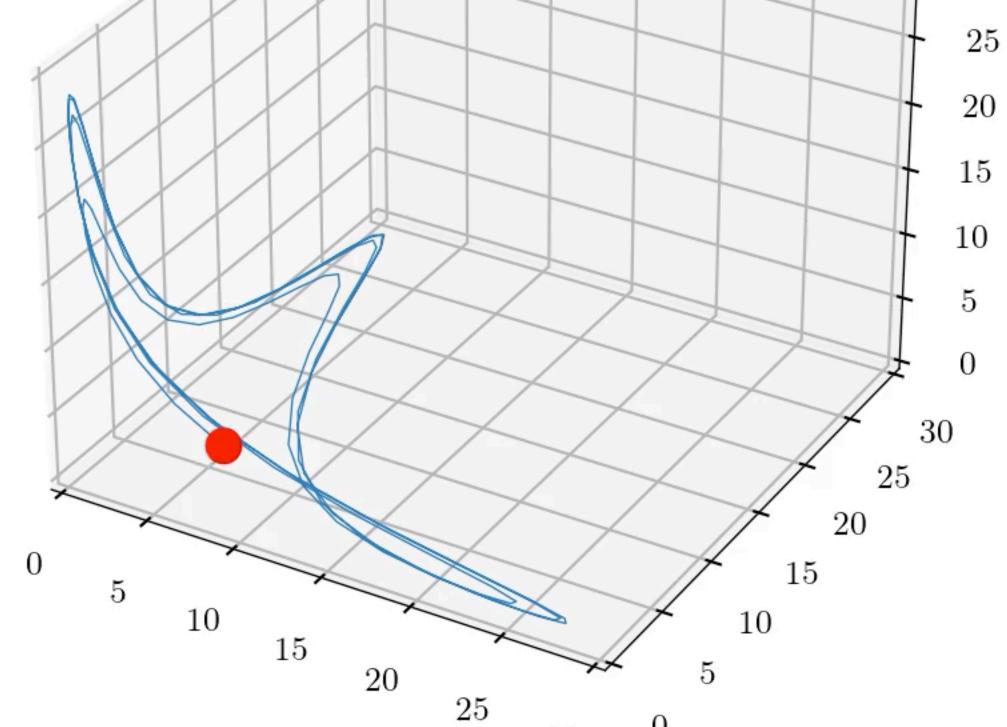
Populations of the three species ultimately equilibrate to the relative values predicted by the Boltzmann distribution, but they never stop fluctuating, and the fluctuations are big if the total numbers are small.

Boring ODEs

```
from mpl toolkits.mplot3d import Axes3D
param = [50, 0, 0.2, 2]
# Initial conditions.
y0 = [1.5, 0.5, 1, 1.5, 2, 2]
# Set number of points and frames to use, frame rate.
num = 200
max frames = 80
rate = 20
# Times at which solution to ODE will be evaluated.
times = np.arange(0, num)
# Function to use with odeint: dy/dt = F(y,t)
def repressilatorVF(y, t):
   # input: y = array of 6 dynamical variables
   # returns: vector field VF of derivatives
    VF = np.zeros(6)
    VF[0] = -y[0] + param[0]/(1.+y[5]**param[3])+ param[1];
    VF[1] = -y[1] + param[0]/(1.+y[3]**param[3])+ param[1];
    VF[2] = -y[2] + param[0]/(1.+y[4]**param[3])+ param[1];
    VF[3] = -param[2]*(y[3]-y[0]);
    VF[4] = -param[2]*(y[4]-y[1]);
    VF[5] = -param[2]*(y[5]-y[2])
    return VF
#%% Solve the ODE.
y = odeint(repressilatorVF, y0, times)
```



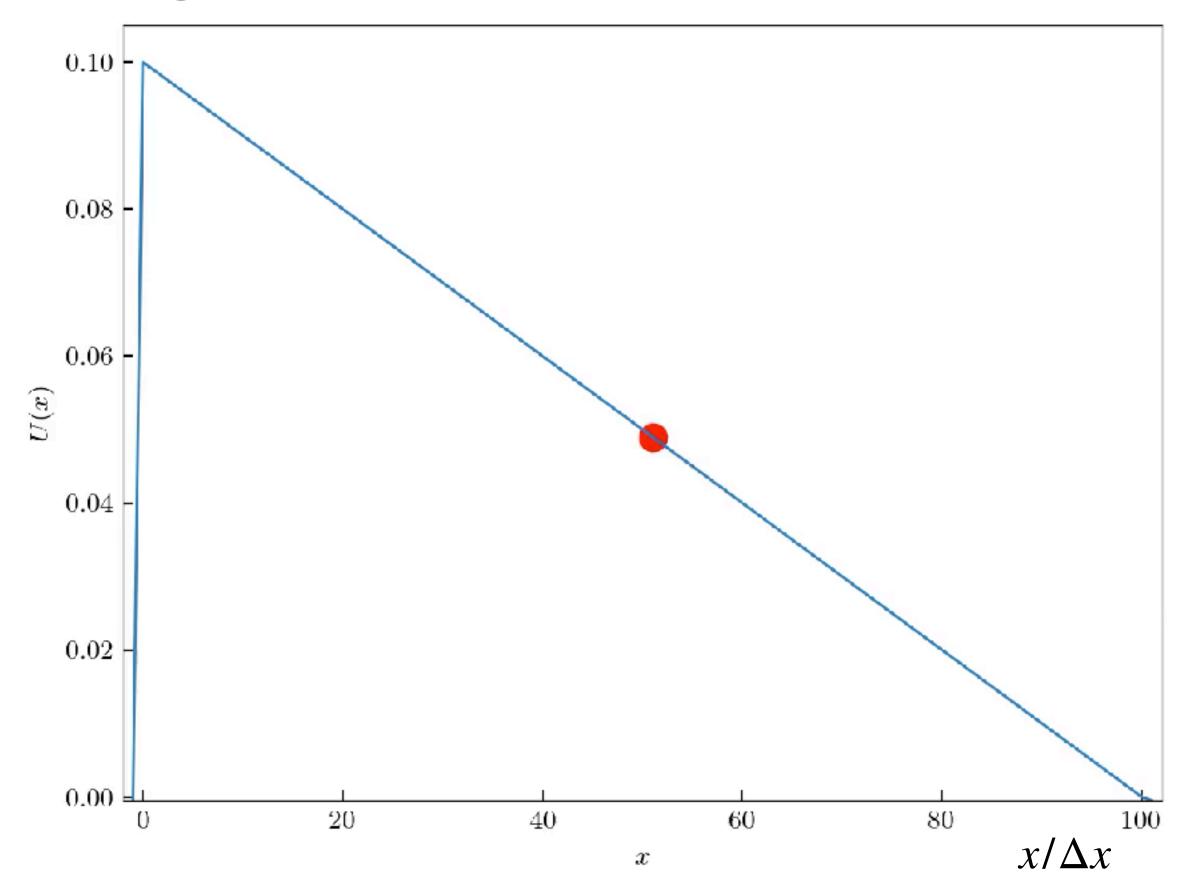
Thrilling ODEs



Make some sort of 3D animated line or point plot of your own (maybe an explicit function, not the solution to an ODE). This time, the key is that you must create the axes with

```
ax3d = plt.figure().add_subplot(projection = '3d')
... then initialize the moving point:
my_point, = ax3d.plot([], [], [], 'ro', ms=9)
... then in the rendering function:
my_point.set_data_3d((y[now, 0],), (y[now, 1],), (y[now, 2],))
```

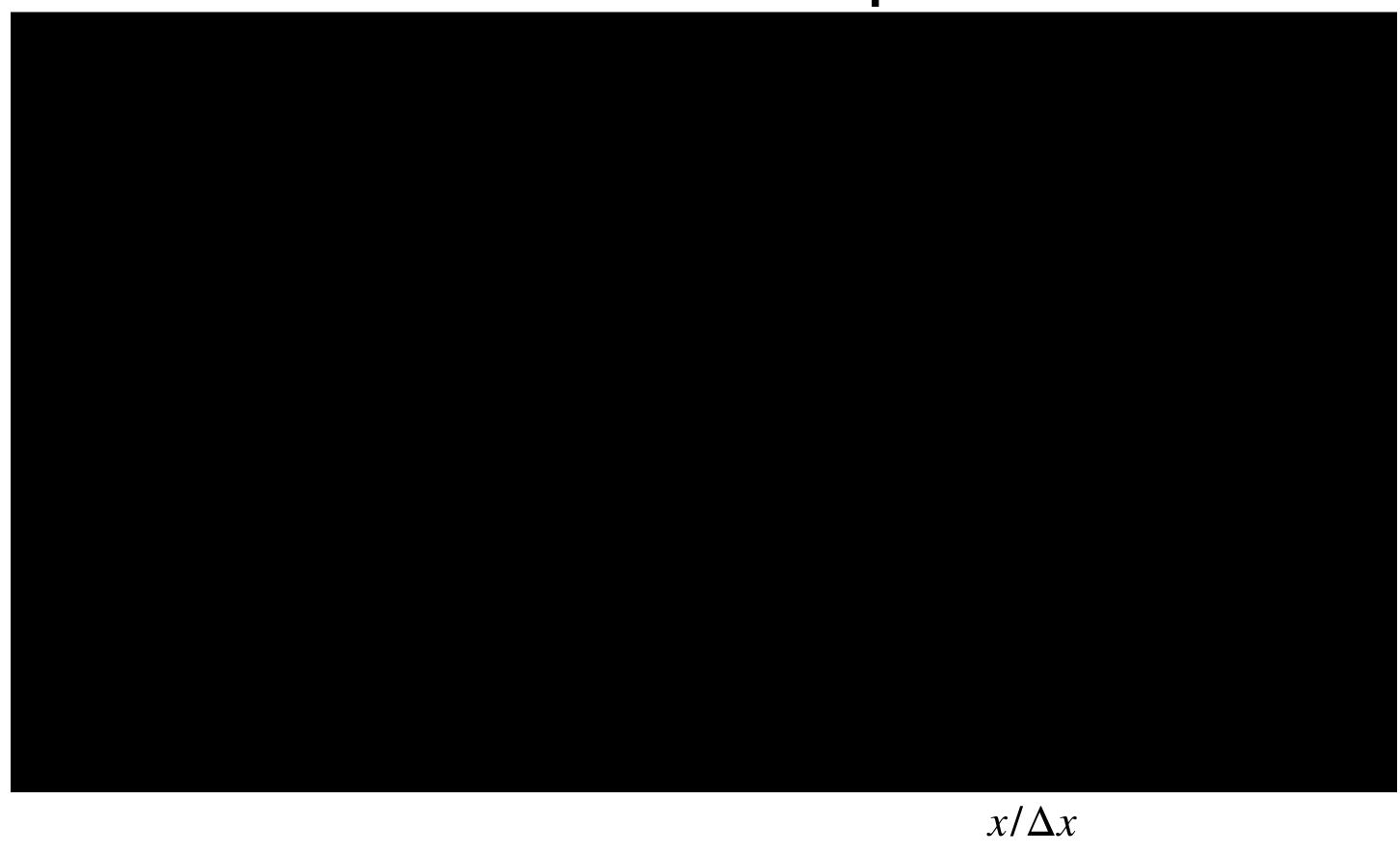
Falling off a cliff



The walker is not "trying to get out." It doesn't even "know" that there is a way out.

The walker is not "creeping toward the exit." It's just blundering around, and eventually it stumbles upon the exit. Meanwhile it often "wastes" lots of time on excursions in the "wrong" direction.

Brownian in a trap: The movie

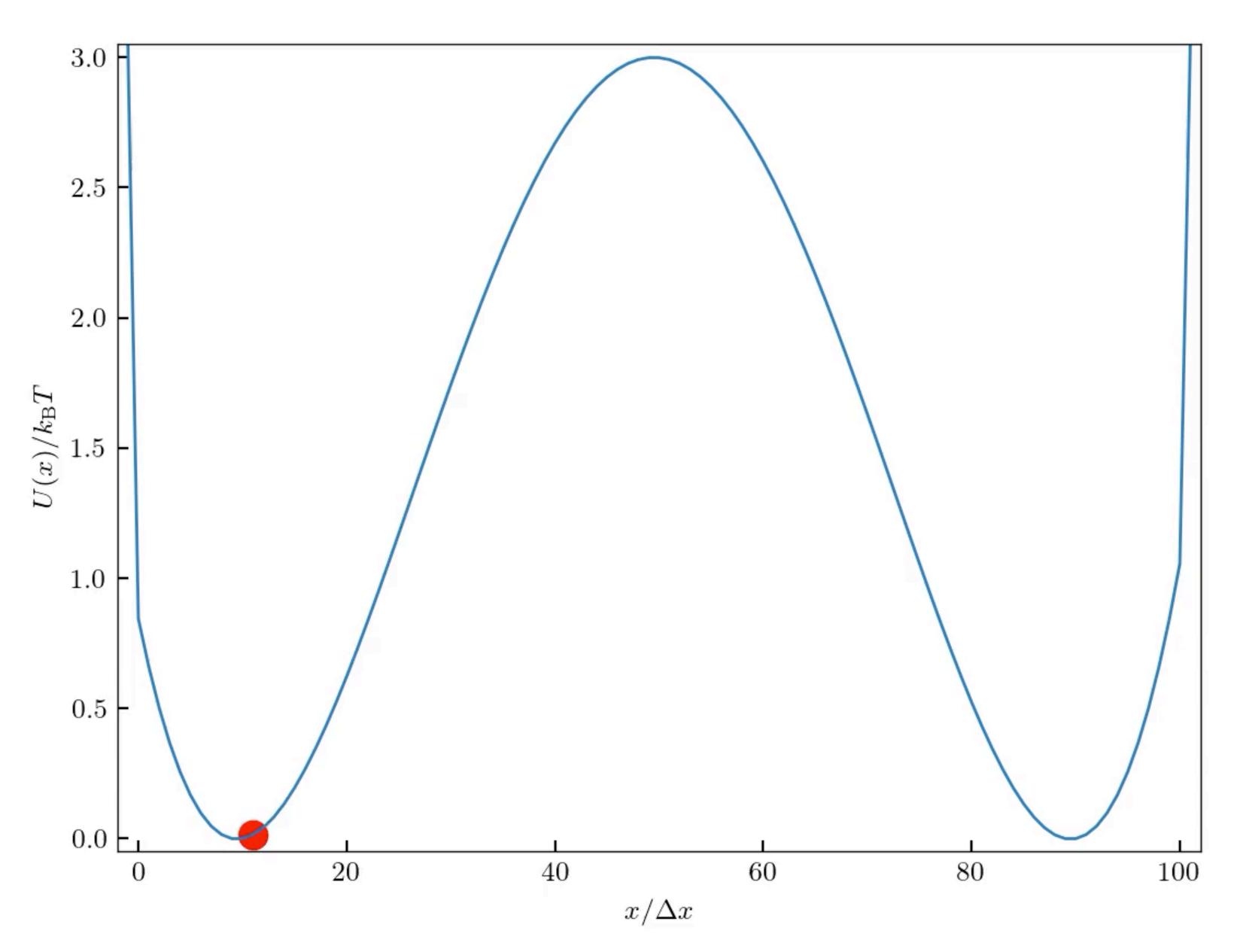


The walker is not "trying to get out." It doesn't even "know" that there is a way out.

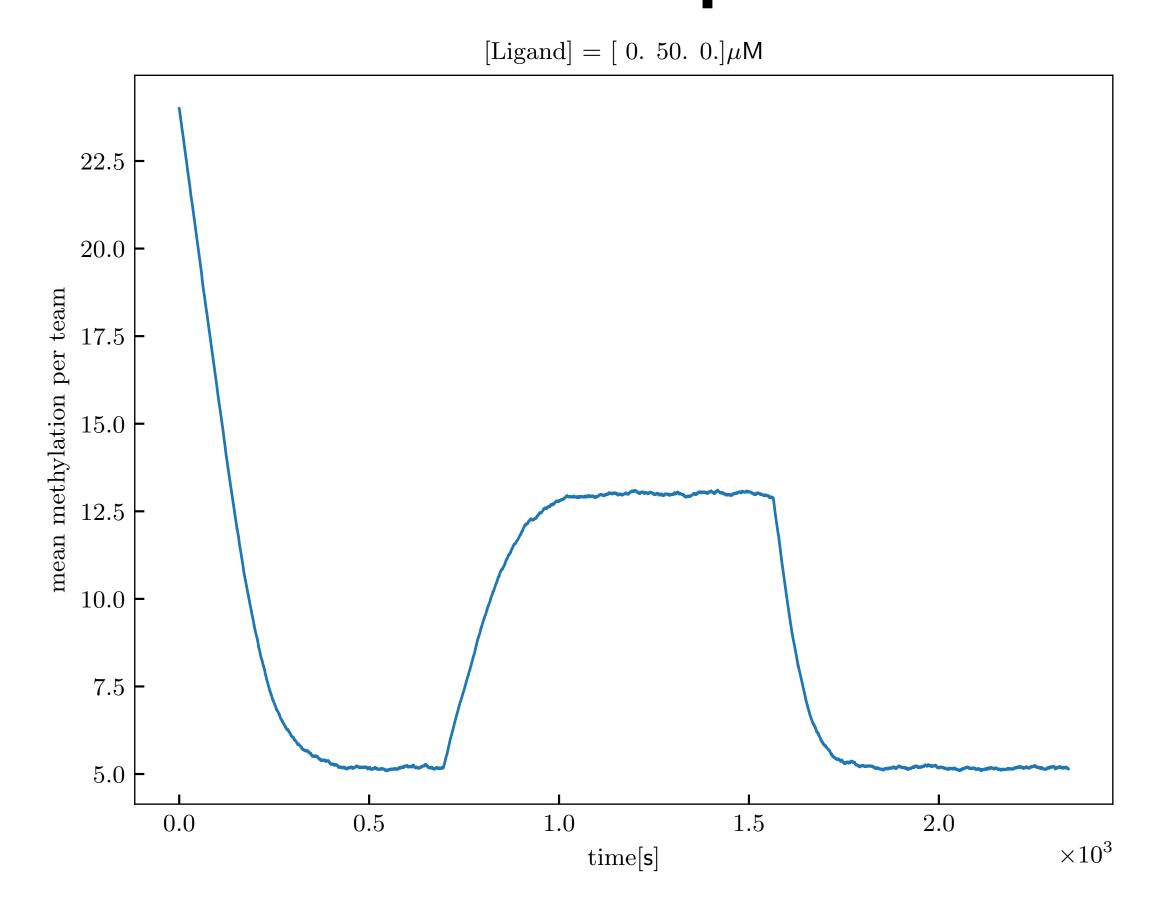
The walker is not "creeping toward the exit." It's just blundering around, and eventually it stumbles upon the exit. Meanwhile it often "wastes" lots of time on excursions in the "wrong" direction.

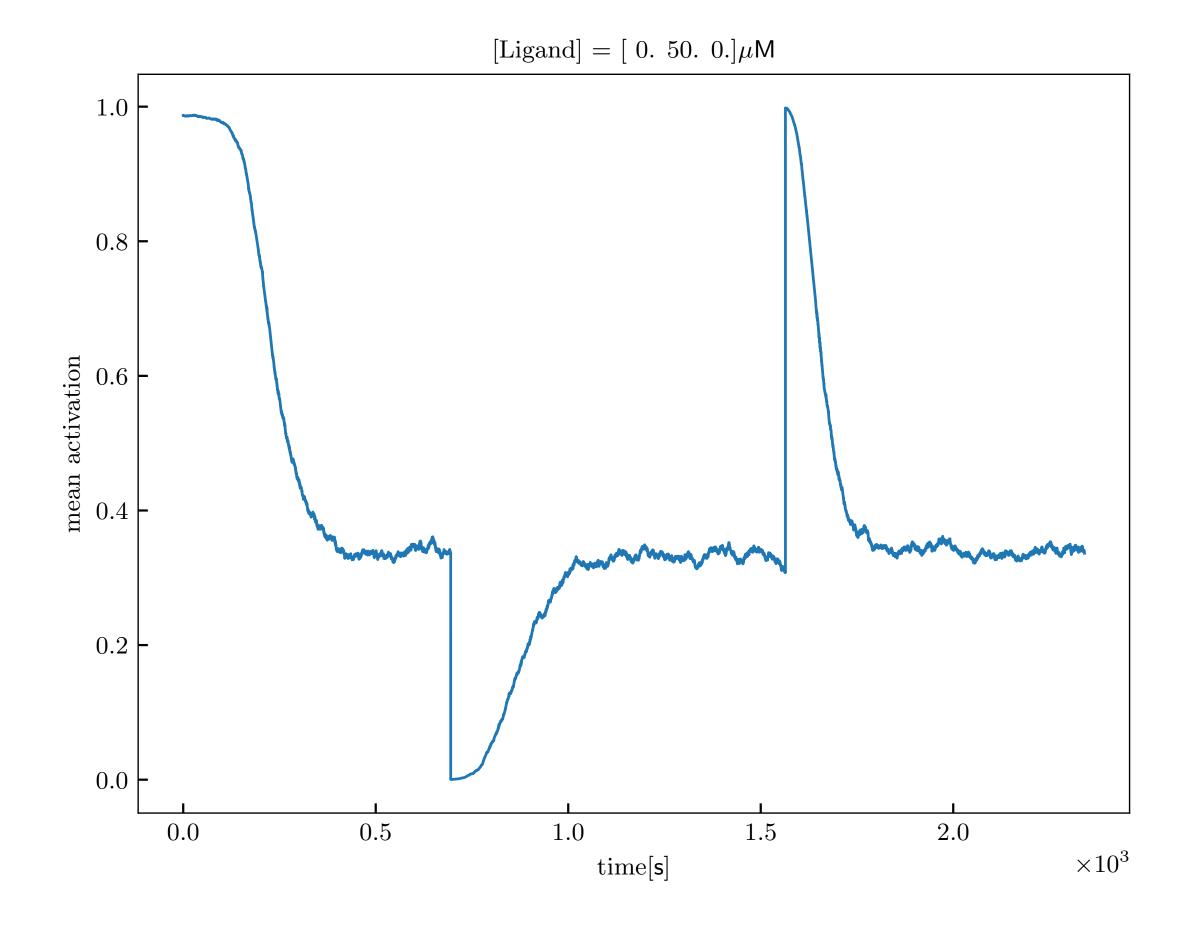
https://www.physics.upenn.edu/biophys/PMLS2e/Media/brownianTrapSim/escapeTraj.mp4

Isomerization as a double well

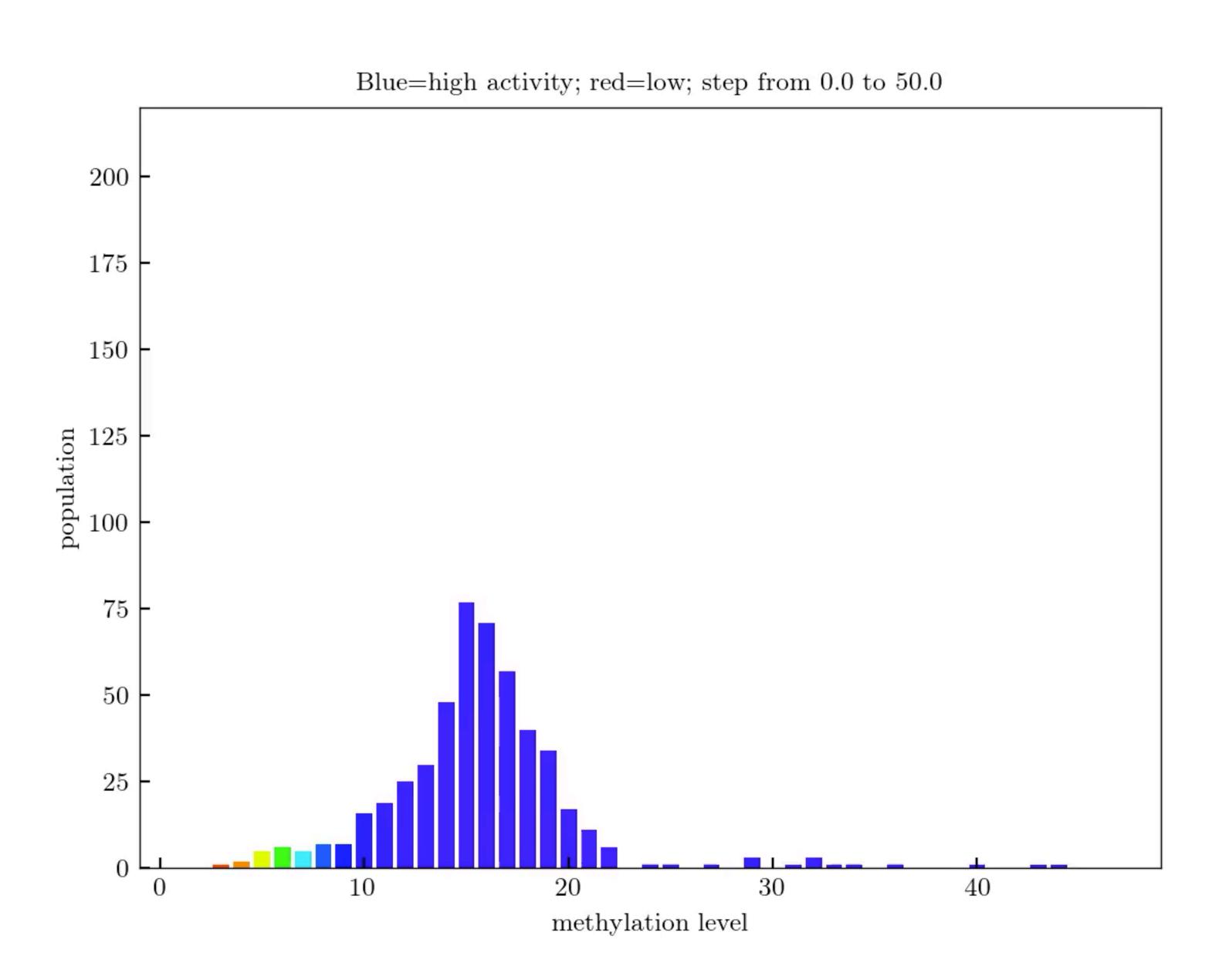


Adaptation in chemotaxis





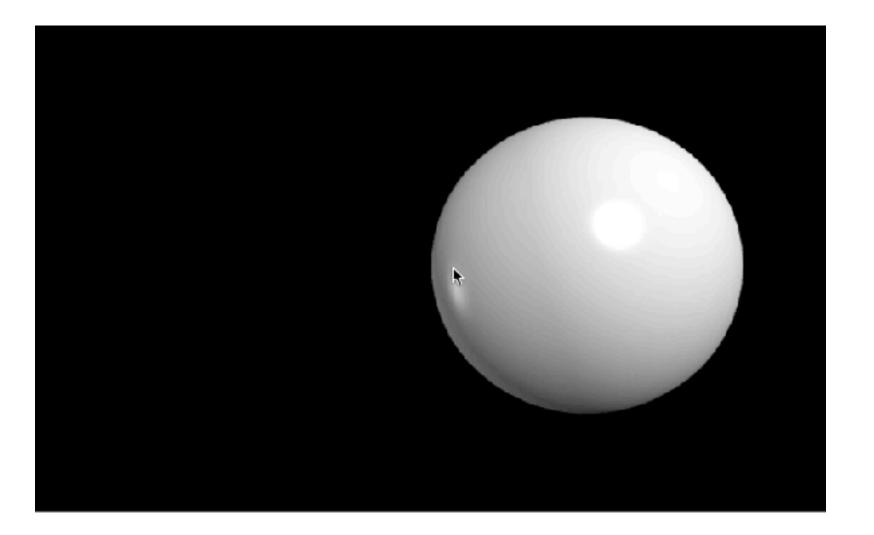
Story about adaptation in chemotaxis



Stories about 3D objects

\$ conda install conda-forge::vpython





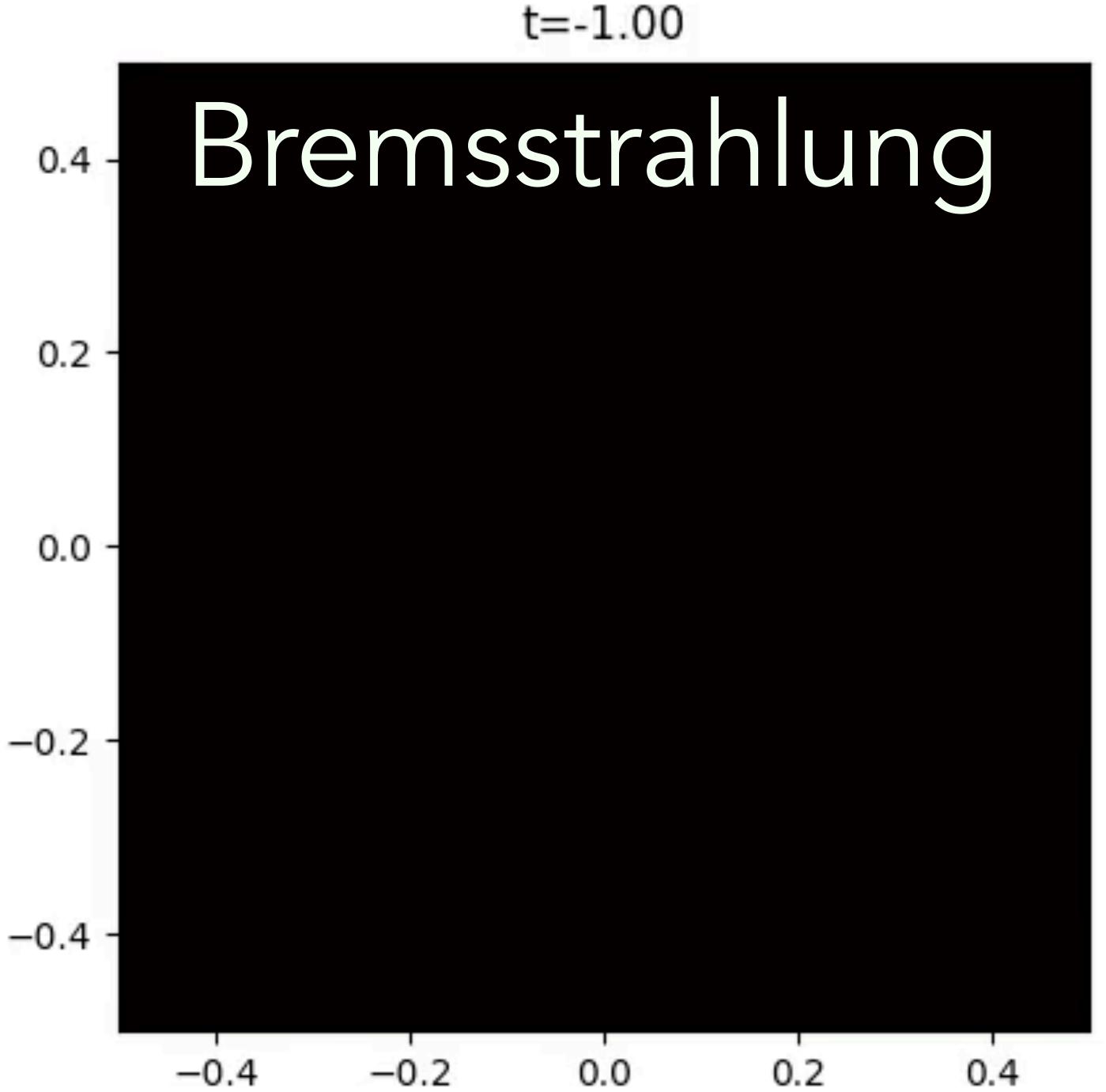
Just a few lines of code succeed in reproducing realistic behavior: See code flipper.ipynb.

Courtesy Adam J Simon; see Adam Simon and Albert Libchaber. Escape and synchronization of a Brownian particle. Phys. Rev. Lett. 68, 3375 (1992) https://www.physics.upenn.edu/biophys/PMLS2e/Media/brownian/BeadJump.m4v

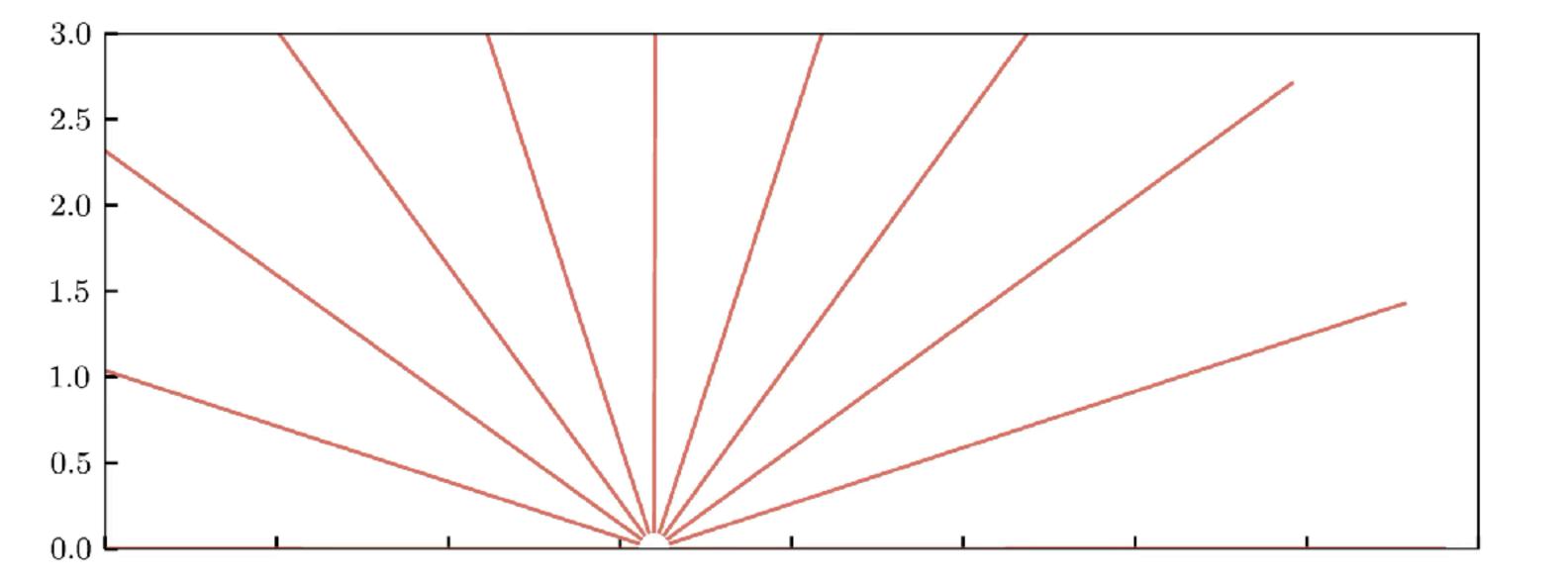
Ray tracing for that meme-worthiness

VPython can export PovRay files; then free PovRay app can render them with ray-tracing; then ffmpeg can stitch the frames into a video.

Chen, K. Y., Zuckerman, D. M., & Nelson, P. C. (2020). Stochastic simulation to visualize gene expression and error correction in living cells. The Biophysicist, 1(1), Art. 1. https://doi.org/10.35459/tbp.2019.000101. Code: https://github.com/NelsonUpenn/PNelson_code

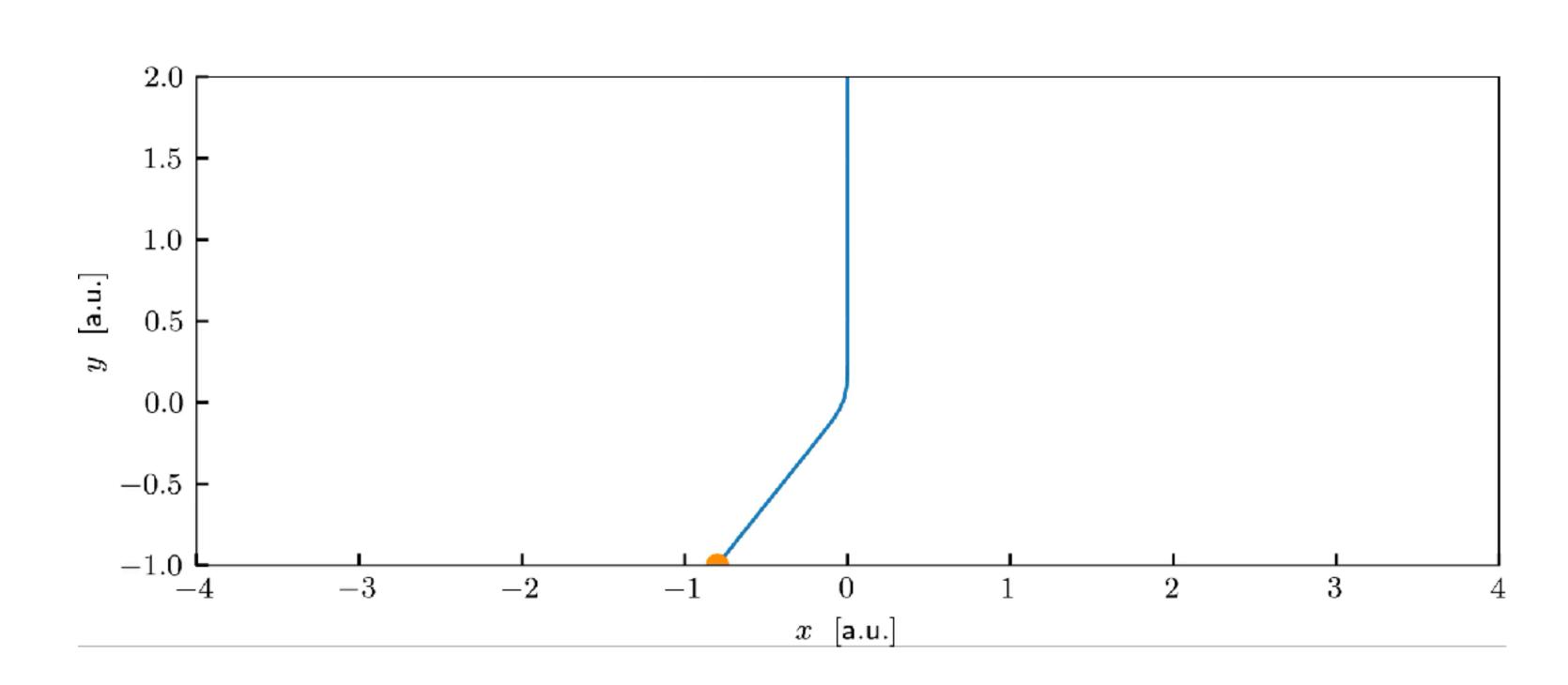


Bremsstrahlung



Lower: World-line of a particle in uniform motion along x that rapidly comes to a stop.

Upper: Resulting electric field lines.



Attack of the flying bananas

A circular loop of wire in the plane perp to the screen pierces the screen at the black dot.
(There is a mirror-image to the left of this figure.)
Blue curves are electric field lines resulting when alternating current flows in the loop.

