Lecture 6

We will discusss visual package briefly.

To install on Mac, go to vpython.org

Follow instructions to download Python-2.7.9 + then VPython-Mac-Py 2.7-6.11

This installs an older version of Python that is compatible w/ vpython/visual

This can run alongside Anaconda
Use Spyder for Python 3.4
+ VIDLE for visual/python 2.7

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Bring up 0-sphere.py

simple program to plot a sphere

can change the size & position of sphere w/

sphere(radius = 0.5, pos = [1.0, -0.2, 0.0])

can draw many spheres &

change their colors.

Bring up 1-spheres.py

You can change properties of a sphere after creating it. Use

s = sphere()

creates a variable for the sphere. (really an object)

can change properties w/
s.radius = 0.5
s.color = color.blue
can use these to make animations

can also draw other objects besides spheres, including

box
cone
cylinder
pyramid
arrow

can change properties of the screen window w/ display function

many options for this function like foreground color, location of "camera", "camera angle",
can make a variable d = display() to
change properties later on

can make animations,
which might be helpful for
visualizing physical systems

could do, e.g.,

```
from visual import sphere
s = sphere(pos=[0,0,0])
s.pos = [1,4,3]
```

however, computer will be so fast
that you won't notice the change

to slow down, use the
rate function

rate(x) tells Python to wait
$1/x$ seconds since previous
time rate was called.

Bring up 3-revolve.py

Move on to Chap. 5

Integration

Might not be possible to evaluate integrals by hand.

We can instead evaluate w/ computer to get approximate results.

Simplest rule is trapezoidal rule

Show 4-trapezoidal.png

Given function $f(x)$ &

suppose we want integral from $x=a$ to $x=b$

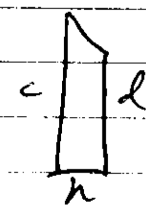
$$I(a,b) = \int_a^b f(x)\, dx$$

divide area under curve into trapezoids

Divide $[a,b]$ into N slices

so each slice has width $h = (b-a)/N$

recall area of trapezoid is



$= \frac{c+d}{2} h$

RHS of kth slice occurs @ $a+kh$

& LHS @ $a+kh-h = a + (k-1)h$

$\Rightarrow$ area of trapezoid for this slice is

$$A_k = \frac{1}{2} h \left[f(a+(k-1)h) + f(a+kh) \right]$$

So approximation for integral is

$$I(a,b) \simeq \sum_{k=1}^{N} A_k$$

$$= \frac{1}{2} h \sum_{k=1}^{N} \left[f(a+(k-1)h) + f(a+kh) \right]$$

$$= h\left[\tfrac{1}{2}f(a) + f(a+h) + f(a+2h) + \dots + f(a+(N-1)h) + \tfrac{1}{2}f(b)\right]$$

$$= \underbrace{h\left[\tfrac{1}{2}f(a) + \tfrac{1}{2}f(b) + \sum_{k=1}^{N-1} f(a+kh)\right]}_{\text{extended trapezoidal rule}}$$

Example: calculate integral of

$x^4 - 2x + 1$ from $x=0$ to $x=2$

using this rule.

By hand, it works out to

$$\int_0^2 (x^4 - 2x + 1)\,dx = \frac{x^5}{5} - x^2 + x \Big|_0^2$$

$$= \frac{32}{5} - 4 + 2 = \frac{22}{5} = 4.4$$

Bring up 4-trapezoidal.py

try out higher levels of accuracy

Alternative to trapezoidal rule
which can be more accurate
is Simpson's rule.

trapezoidal rule uses straight-line
segments for approximation, but we
can instead use curves.

Simpson's rule fits w/ quadratic
curves

Show 5-simpson.png

We require 3 points to specify
a quadratic (not just 2 as
w/ a line)

so fit a quadratic to pairs of
adjacent slices

Suppose integrand is $f(x)$ & spacing is
h

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Suppose three points are @

$-h$, 0, $+ h$

Fitting a quadratic

$Ax^2 + Bx + C$ through these points gives

$$f(-h) = Ah^2 - Bh + C$$

$$f(0) = C$$

$$f(h) = Ah^2 + Bh + C$$

Solving these equations for A, B, C gives

$$A = \frac{1}{h^2} \left\{ \tfrac{1}{2} f(-h) - f(0) + \tfrac{1}{2} f(h) \right\}$$

$$B = \frac{1}{2h} \left[f(h) - f(-h) \right]$$

$$C = f(0)$$

+ area under curve from $-h$ to h is approximated by area under quadratic

$$\int_{-h}^{h} (Ax^2 + Bx + C)\, dx$$

$$= \frac{2}{3} Ah^3 + 2Ch$$

$$= \frac{1}{3} h \left[f(-h) + 4f(0) + f(h) \right]$$

This is the Simpson rule.

Approximates area under two adjacent slices.

Need an even # of slices for this to work

Approximate value of an integral over $[a,b]$ is

$$I(a,b) \simeq \frac{1}{3} h \left[f(a) + 4f(a+h) + f(a+2h) \right]$$
$$+ \frac{1}{3} h \left[f(a+2h) + 4f(a+3h) + f(a+4h) \right]$$
$$+ \dots + \frac{1}{3} h \left[f(a+(N-2)h) + 4f(a+(N-1)h) + f(b) \right]$$

$$= \frac{1}{3} h \left[f(a) + 4 f(a+h) + 2 f(a+2h) + 4 f(a+3h) + \dots + f(b) \right]$$

$$= \frac{1}{3} h \left[f(a) + f(b) + 4 \sum_{\substack{k \text{ odd} \\ 1,\dots,N-1}} f(a+kh) + 2 \sum_{\substack{k \text{ even} \\ 2,\dots,N-2}} f(a+kh) \right]$$

extended Simpson's rule

Bring up 5-simpson.py

What is the error associated w/ trapezoidal rule?

Main source of error is not rounding error but error in approximating integral (b/c we're calculating an approximation to integrand)

How big is the error?

We can quantify w/ some simple tricks

Recall trapezoidal rule gives

$$\int_a^b f(x)\,dx = I(a,b) \simeq h\left[\tfrac{1}{2}f(a) + \tfrac{1}{2}f(b) + \sum_{k=1}^{N-1} f(a+kh)\right]$$

Let $x_k = a + kh$

Consider slice of integral between x_{k-1} & x_k

Perform Taylor series expansion of $f(x)$ about x_{k-1}

so that

$$f(x) = f(x_{k-1}) + (x - x_{k-1}) f'(x_{k-1}) + \frac{(x-x_{k-1})^2}{2} f''(x_{k-1}) + \cdots$$

Integrate this from x_{k-1} to x_k to get

$$\int_{x_{k-1}}^{x_k} f(x)\,dx = f(x_{k-1}) \int_{x_{k-1}}^{x_k} dx + f'(x_{k-1}) \int_{x_{k-1}}^{x_k} (x - x_{k-1})\,dx + \frac{1}{2} f''(x_{k-1}) \int_{x_{k-1}}^{x_k} (x - x_{k-1})^2 + \cdots$$

Make substitution $u = x - x_{k-1}$ so that

$$\int_{x_{k-1}}^{x_k} f(x)\,dx = f(x_{k-1}) \int_0^h du + f'(x_{k-1}) \int_0^h u\,du + \frac{1}{2} f''(x_{k-1}) \int_0^h u^2\,du + \cdots$$

$$= h\, f(x_{k-1}) + \frac{1}{2} h^2 f'(x_{k-1})$$

$$(*) \quad + \frac{1}{6} h^3 f''(x_{k-1}) + \underbrace{O(h^4)}_{\text{higher order terms}}$$

Can also expand around $x = x_k$
& integrate from x_{k-1} to x_k

$$\int_{x_{k-1}}^{x_k} f(x)\,dx = h f(x_k) - \tfrac{1}{2}h^2 f'(x_k) + \tfrac{1}{6}h^3 f''(x_k) - O(h^4) \qquad (**)$$

Take average of (*) & (**) to get

$$\int_{x_{k-1}}^{x_k} f(x)\,dx = \tfrac{1}{2}h\left[f(x_{k-1}) + f(x_k)\right] + \tfrac{1}{4}h^2\left[f'(x_{k-1}) - f'(x_k)\right] + \tfrac{1}{12}h^3\left\{f''(x_{k-1}) + f''(x_k)\right\} + O(h^4)$$

Now sum this over all slices to get

$$(***) \quad \int_a^b f(x)\,dx = \sum_{k=1}^{N} \int_{x_{k-1}}^{x_k} f(x)\,dx$$

$$= \tfrac{1}{2}h \sum_{k=1}^{N}\left\{f(x_{k-1}) + f(x_k)\right\} + \tfrac{1}{4}h^2\left[f'(a) - f'(b)\right] + \tfrac{1}{12}h^3 \sum_{k=1}^{N}\left[f''(x_{k-1}) + f''(x_k)\right] + O(h)$$

1st sum is trapezoidal rule

All other terms correspond to error in approximation

Second term is nice - many terms cancel and we are left w/ only first & last terms

Observe that third term is trapezoidal rule approximation to $f''(x)$ over interval from a to b.

So using same formula but substituting $f(x) \to f''(x)$, we find that

$$\int_a^b f''(x)\,dx = \frac{1}{2}h \sum_{k=1}^{N} \left[f''(x_{k-1}) + f''(x_k)\right] + O(h^2)$$

Multiply by $\frac{1}{6}h^2$ & rearrange to find that

$$\frac{1}{12} h^3 \sum_{k=1}^{N} [f''(x_{k-1}) + f''(x_k)]$$

$$= \frac{1}{6} h^2 \int_a^b f''(x)\,dx + O(h^4)$$

$$= \frac{1}{6} h^2 [f'(b) - f'(a)] + O(h^4)$$

Now substitute back into (***) to get

$$\int_a^b f(x)\,dx = \frac{1}{2} h \sum_{k=1}^{N} \{f(x_{k-1}) + f(x_k)\}$$

$$+ \frac{1}{12} h^2 \{f'(a) - f'(b)\} + O(h^4)$$

To leading order in h, we

see that error from trap. rule is

$$\varepsilon = \frac{1}{12} h^2 [f'(a) - f'(b)]$$

called the Euler - MacLaurin formula

$\Rightarrow$ trapezoidal rule is first-order integration rule, accurate up to terms proportional to h & leading-order approx. error is order h^2

1^{st}-order rule is accurate to $O(h)$ + has error $O(h^2)$.

There is also a rounding error

recall that rounding error is
Cx where x is value of #
+ C is machine precision,
which is $C \approx 10^{-16}$

can make h smaller but then there is a limit to increasing accuracy due to rounding error.

decreases in h help only to the point at which approx. error + rounding error are equal, which is

$$\frac{1}{12} h^2 \left[f'(a) - f'(b) \right] = C \int_a^b f(x)\,dx$$

Solve for h to get

$$h \simeq \sqrt{\frac{12 \int_a^b f(x)\,dx}{f'(a) - f'(b)}}\; C^{1/2}$$

set $h = (b-a)/N$ to get

$$N \simeq (b-a) \sqrt{\frac{f'(a) - f'(b)}{12 \int_a^b f(x)\,dx}}\; C^{-1/2}$$

So, e.g., if all factors except C are around 1 then

$$N \simeq 10^8$$

But this is a bit large, & would be wiser to use smaller N w/ more accurate rule like Simpson rule.