Computational Methods Exercise - Solution Release

CONTENTS

1	Preface	1		
2 Contemporary Trends in Atmospheric CO ₂				
3	Compartmental Model of the Global Carbon Cycle 3.1 Problem 1	14		
4	merical Methods			
5	Model Application to Observed Atmospheric CO2 Concentrations 5.1 20th Century Emissions 5.2 Looking Towards the Future 5.3 Projection of future climate change using RCP scenarios	37		
6	Code Samples 6.1 Compartmental Carbon Cycle Model			

CHAPTER

ONE

PREFACE

This is a reference solution for the **12.806 Computational Modeling Exercise**, including versions of required and suggested figures for reference and all code used to produce the solution. This solution was implemented in Python, leaning on several widely-used and actively developed and maintained scientific and numerical libraries.

For convenience, we'll use two very powerful libraries from the scientific Python stack:

- NumPy a numerical framework for Python centered around an *n*-dimensional array object; includes many useful mathematical functions.
- pandas an analysis package based on data tables; allows you to quickly organize tabular data and run common statistics and analysis on them.

Additionally, we'll need to generate some plots, so we'll use standard Python visualization libraries:

- matplotlib Matlab-like visualization library
- seaborn extension to matplotlib which generates quick statistical plots when data is packaged into pandas data structures; additionally includes aesthetic tweaks which greatly improve the matplotlib basics

Finally, to read the Excel spreadsheet data source in the final part of this notebook, you'll need the xlrd package, which you can install by invoking:

```
$ pip install xlrd
```

All of the snippets shown here are culled from a companion Jupyter Notebook which you can modify and run on your own personal machine.

CONTEMPORARY TRENDS IN ATMOSPHERIC CO2

We'll start by downloading the monthly mean CO₂ data, using a shell command in the cell below.

```
wget ftp://aftp.cmdl.noaa.gov/products/trends/co2/co2_mm_mlo.txt .
```

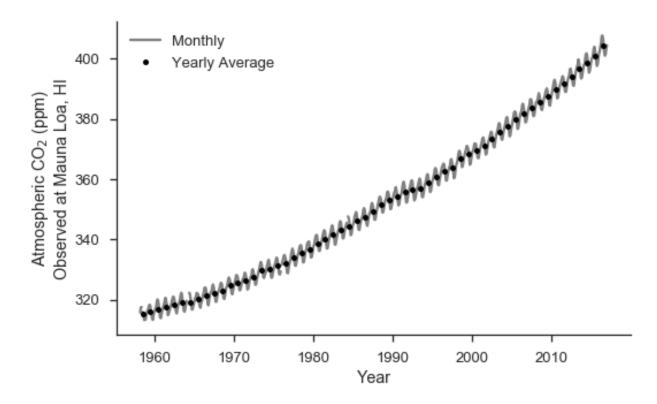
```
--2017-013-30 14:27:52-- ftp://aftp.cmdl.noaa.gov/products/trends/co2/
⇒co2_mm_mlo.txt
          => 'co2_mm_mlo.txt'
Resolving aftp.cmdl.noaa.gov... 140.172.200.31
Connecting to aftp.cmdl.noaa.gov|140.172.200.31|:21... connected.
Logging in as anonymous ... Logged in!
==> SYST ... done.
                    ==> PWD ... done.
==> TYPE I ... done. ==> CWD (1) /products/trends/co2 ... done.
==> SIZE co2_mm_mlo.txt ... 49083
==> PASV ... done.
                     ==> RETR co2_mm_mlo.txt ... done.
Length: 49083 (48K) (unauthoritative)
100%[======>] 49.083
                                                         223KB/s
\rightarrowin 0.2s
2017-01-30 14:27:54 (223 KB/s) - 'co2 mm mlo.txt' saved [49083]
--2017-01-30 14:27:54-- http://./
Resolving .... failed: nodename nor servname provided, or not known.
wget: unable to resolve host address '.'
FINISHED --2017-01-30 14:27:54--
Total wall clock time: 2.6s
Downloaded: 1 files, 48K in 0.2s (223 KB/s)
```

Read in the table using Pandas' I/O functions. We'll independently supply column names and have it automatically sniff out the appropriate whitespace separation between columns. Furthermore, we'll mask missing values, and construct a pivot-table broken down into a multi-index based on year and month (which will be useful later on for analysis). Note that we didn't need to delete the original metadata header to the input data - using the **comment** argument to read_table(), we can instruct Pandas to ignore those lines.

From the data, we'll plot the monthly mean data alongside yearly-mean data that we've computed by aggregated and averaging the pivot-table data by year. Note that we shift the index of the yearly data by half of a year, just for plotting purposes (so it lines up with the middle of the year).

We'll wrap the plotting mechanics in its own function so that we can use this as a base for future plots with additional analysis later on.

```
fig = plt.figure(figsize=(8, 5))
ax = fig.add_subplot(111)
def mauna_loa_plot(ax):
    """ Wrapper for basic Mauna Loa plot, so we can plot additional
    curves later on """
    ax.plot(mauna_loa.decimal_date, mauna_loa.average,
            '-', color='grey', label="Monthly")
    ax.plot(mauna_loa_yearly.index + 0.5, mauna_loa_yearly.average,
            'ok', ms=5, label='Yearly Average')
    ax.legend(loc='upper left')
    ax.set_xlabel("Year")
    ax.set_ylabel("Atmospheric CO$_2$ (ppm) \nObserved at Mauna Loa, HI
" )
   sns.despine()
    return ax
ax = mauna_loa_plot(ax)
```



Now we need to generate polynomial fits to the data. In other terms, we want to compute the coefficients in equations like

$$P_1(t) = a + bt$$

and

$$P_2(t) = a + bt + ct^2$$

such that we minimize the residual between the estimated data and the observations,

$$\sum_{i=1}^{n} \left| P_i(t_i) - y(t_i) \right|$$

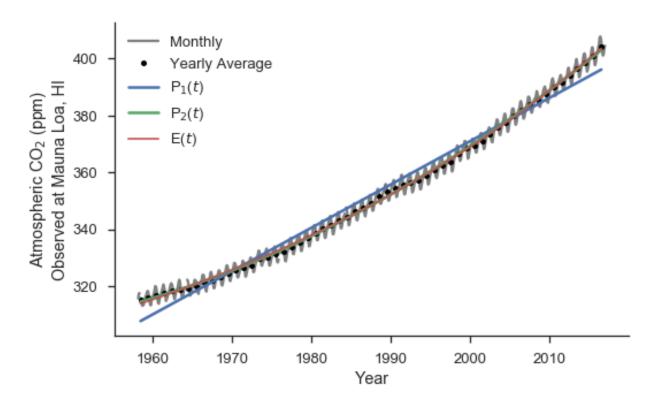
For the polynomials, we can use the built-in <code>polyfit</code> and <code>poly1d</code> tools from NumPy, which will take care of setting up the polynomials and evaluating them based on the resulting coefficients we compute. However, for the exponential fit, we'll use a helper function from SciPy's <code>optimize</code> package called <code>curve_fit</code>, which allows us to define an arbitrary functional form. The package will take care of the non-linear least squares fitting (done via Levenberg-Marquardt in this case). Note that we could alternatively take the logarithm of the exponential fit, which produces a linear equation we can fit using traditional least-squares.

```
xi = mauna_loa_yearly.index + 0.5
yi = mauna_loa_yearly.average
```

```
## 1st degree
p_1 = np.poly1d( np.polyfit(xi, yi, 1) )
print "First order -"
print p_1
## 2nd degree
p_2 = np.poly1d(np.polyfit(xi, yi, 2))
print "Second order -"
print p_2
## Exponential
from scipy.optimize import curve_fit
def exp_func(x, a, b, c):
   x_{off} = x - xi[0] # we re-base x at 0 for numerical
                      # purposes
    return a + b*np.exp(-c*x_off)
coeff_opt, pcov = curve_fit(exp_func, xi, yi)
exf = lambda x: exp_func(x, *coeff_opt)
print "Exponential -"
print \{0:.2e\} + \{1:.2e\} exp(\{2:+.2e\}*(t - 1850))".format(*coeff_opt)
fig = plt.figure(figsize=(8,5))
ax = fig.add_subplot(111)
mauna_loa_plot(ax)
ax.plot(xi, p_1(xi), lw=2.5, label="P$_1$($t$)")
ax.plot(xi, p_2(xi), lw=2.5, label="P$_2$($t$)")
ax.plot(xi, exf(xi), lw=2,
        label="E(\$t\$)", alpha=.8)
ax.legend(loc='upper left')
```

```
First order -

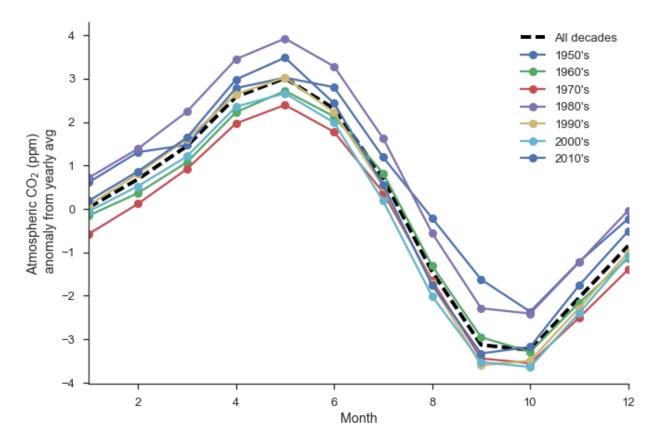
1.524 x - 2677
Second order -
2
0.0124 x - 47.77 x + 4.63e+04
Exponential -
2.56e+02 + 5.76e+01 exp(-1.62e-02*(t - 1850))
```



Let's de-trend the data using the 2nd-order polynomial $P_2(t)$, which produces a rather good fit. Then, we'll average the seasonal cycle in terms of an anomaly for each decade using a split-apply-combine operation, and then plot the annual cycle for each decade.

```
mauna_loa['average_detrend'] = \
   mauna_loa['average'] - p_2(mauna_loa['decimal_date'])
mauna_loa['decade'] = \
    np.floor((mauna_loa['year'] - 1900)/10.)
monthly = mauna_loa.groupby('month')
ml_mo_cycle = monthly.aggregate(np.mean)
plt.plot(ml_mo_cycle.index, ml_mo_cycle['average_detrend'],
         '--k', label='All decades', lw=4)
decade_groups = mauna_loa.groupby(['decade', 'month'])
ml_dec_cycle = decade_groups.aggregate(np.mean)
decades = ml_dec_cycle.index.levels[0]
for decade in decades:
   ml_dec = ml_dec_cycle.loc[decade]
   plt.plot(ml_dec.index, ml_dec['average_detrend'],
             marker='o', label="%4d's" % (1900+decade*10,))
plt.legend(loc='upper right')
plt.xlim(1, 12)
```

```
plt.xlabel('Month')
plt.ylabel('Atmospheric CO$_2$ (ppm) \n anomaly from yearly avg')
sns.despine()
```



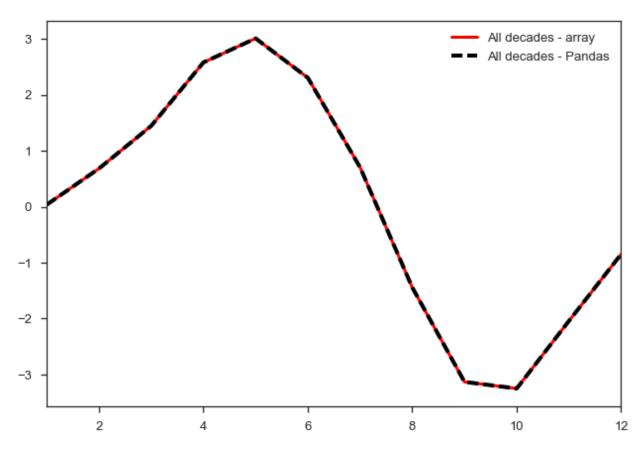
The above calculation gives a peak into how powerful Pandas (and similar libraries) are. The first two lines of the above cell respectively (1) de-trend the data, and (2) calculate what decade a given value takes place in. Then, we go on to group all the data with like decades together, then with like months in each decade, and compute our analysis that way. If we were more clever, we could've assigned a datetime-like index and automatically inferred these values from that. It's worthwhile using these sorts of libraries whenever you're doing timeseries analysis!

Just as a reference, suppose we did not have the nifty timeseries and analysis capabilities of a package like Pandas. We could still easily compute the seasonal cycles above, although we'd have to focus our efforts on keeping track of indices inside a big array. Let's do that, focusing on computing the average seasonal anomaly cycle over all the years in the dataset.

Note that we have to do a little bit of index magic to make sure that we sort the right month into the right place in the array holding the results. Not unbearable, but the Pandas solution is easier and takes all of this into account already.

```
data = mauna_loa.average_detrend[:]
year0 = mauna_loa.year.ix[0]
```

```
month0 = mauna_loa.month.ix[0]
monthly_average = np.zeros(12)
for month in xrange(12):
    monthly_data = data[month::12] # take every 12th element, starting
                                    # at the month we're on
    # Carefully arrange the averages into the proper
    # index in `monthly_average`, based on what the
    # first month in the dataset is
    idx = (month + month0)
    if idx >= 12:
        idx = idx - 12 # You can also say 'idx -= 12', but that's not.
\rightarrow very
                        # Pythonic
   monthly_average[idx-1] = np.mean(monthly_data)
plt.plot(range(1, 13), monthly_average, '-r',
         label="All decades - array", lw=3)
plt.plot(ml_mo_cycle.index, ml_mo_cycle['average_detrend'],
         '--k', label='All decades - Pandas', lw=4)
plt.xlim(1, 12)
plt.legend(loc='upper right')
```



We can now combine the two procedures. In general, if we were fitting some sort of functional model to a complex set of data, we might want to first decompose the model and the data into two separate functions. Then, we could take the linear combination of the two and call that our predictor model. We've implicitly done that already, here, by breaking down the model into a long-term component (the polynomial fits to the yearly data) and a seasonal anomaly on top of the trend.

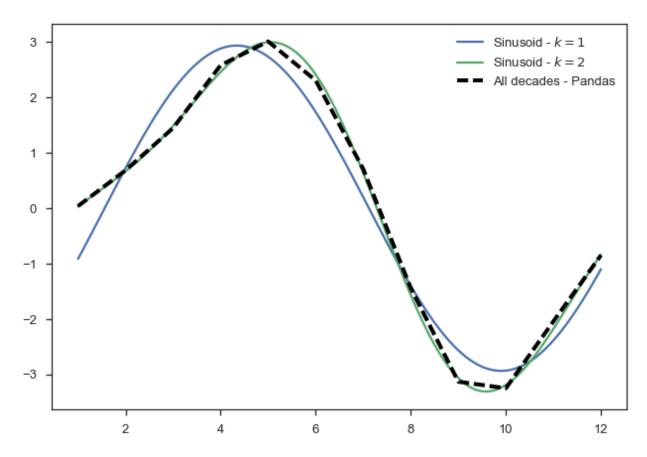
We can formalize this approach by fitting a sine curve of the form

$$y(t) \approx \sum_{k=1}^{n} A_k \sin \frac{2\pi k}{T_k} (t + \phi_k)$$

where A, T, and ϕ are the parameters of interest. Let's fit the seasonal cycle in this way, and try to model the long-term CO_2 record using the combination of the long-term and sesonal components.

Note - We've normalized the month in decimal form at the center of the month (1/12 - 1/24). You don't necessarily have to do this, but it's something to pay attention for later on.

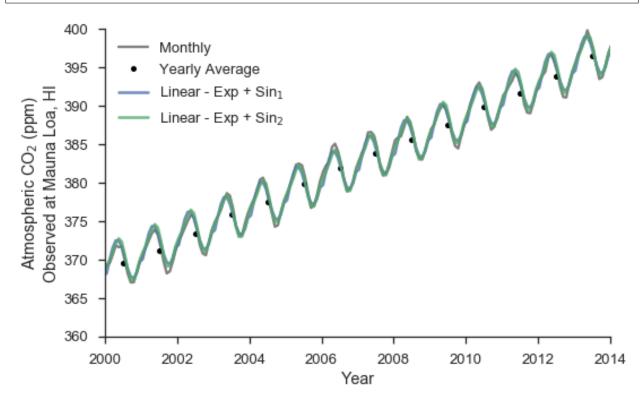
```
## Drop NaNs from the data since it messes up the
## numerical routines
ml_proc = mauna_loa.dropna()
xi = ml_proc.month
xi = (xi/12.) - (1./24.)
yi = ml proc.average detrend
def sin_func_1(x, A, T, phi):
    return A*np.sin((2.*np.pi/T)*(x + phi))
sin_comps_1, _ = curve_fit(sin_func_1, xi, yi)
sin1 = lambda x: sin_func_1(x, *sin_comps_1)
def sin_func_2(x, A1, A2, T1, T2, phi1, phi2):
    return A1*np.sin((2.*np.pi/T1)*(x + phi1)) \
         + A2*np.sin((2.*np.pi/T2)*(x + phi2))
sin_comps_2, _ = curve_fit(sin_func_2, xi, yi)
sin2 = lambda x: sin_func_2(x, *sin_comps_2)
xs = np.linspace(1., 12., 121)
xs_norm = xs/12. - 1./24.
ys1 = sin1(xs\_norm)
ys2 = sin2(xs\_norm)
plt.plot(xs, ys1, label="Sinusoid - $k=1$")
plt.plot(xs, ys2, label="Sinusoid - $k=2$")
plt.plot(ml_mo_cycle.index, ml_mo_cycle['average_detrend'],
         '--k', label='All decades - Pandas', lw=4)
plt.legend()
```



It's straightforward to now combine the long-term trend and the seasonal cycle. We can write a wrapper function to automate the combination for us, and do all the mathemagics that must happen (e.g. month normalizaton, etc)

```
ml_proc = mauna_loa.dropna()
xi = ml_proc.decimal_date.values[:]
yi = ml_proc.average[:]
## Re-do the exponential fit
def exp_func(x, a, b, c):
    x_{off} = x - xi[0] \# we re-base x at 0 for numerical
                      # purposes
    return a + b*np.exp(-c*x_off)
coeff_opt, pcov = curve_fit(exp_func, xi, yi)
exf = lambda x: exp_func(x, *coeff_opt)
def combo(x, k=2):
    # Extract the month in decimal form
    month = x - np.floor(x)
    long_term = exf(x)
    if k == 1:
        seasonal = sin1(month)
```

```
elif k == 2:
        seasonal = sin2 (month)
    else:
        raise ValueError("k = %d not yet defined" % k)
    return long_term + seasonal
fig = plt.figure(figsize=(8,5))
ax = fig.add_subplot(111)
mauna_loa_plot(ax)
ys = [combo(xsi, 1) for xsi in xi]
ax.plot(xi, ys, lw=2.5, label="Linear - Exp + Sin$_1$",
        alpha=0.8)
ys = [combo(xsi, 2) for xsi in xi]
ax.plot(xi, ys, lw=2.5, label="Linear - Exp + Sin$_2$",
        alpha=0.8)
plt.xlim(2000, 2014)
plt.ylim(360, 400)
ax.legend(loc='upper left')
```



We're actually reproducing things incredibly well; we only ever miss out on some peaks to the seasonal cycle (for example in 2002). Of course, we'd need to do some rigorous statistical analysis beyond this to validate that the model isn't just an overfit. But the general steps we used to break down the various components could certainly be repeated elsewhere.

CHAPTER

THREE

COMPARTMENTAL MODEL OF THE GLOBAL CARBON CYCLE

The model was implemented separately (see the appendices). Your mileage may vary in the following portion of the exercise, but in general I'd recommend wrapping your model so that it only takes 1-2 lines of code to initialize the model and then run it, returning all the output you need to analyze the results.

3.1 Problem 1

In the framework of a simple box-model like the one we've written here, one can analyze the lifetime of species in each reservoir by collecting the all the sources and sinks and re-writing the equation in the form

$$\frac{dC}{dt} = \text{Sources} - \text{Sinks}$$

where "Sources" and "Sinks" are all positive and negative terms, respectively, in the original system of ODEs. Neglecting the source term and considering the fact that most of the sinks are going to be represented in the form $k_i X$, we can represent the lifetime as

$$\tau = \frac{X}{\sum_{i=1}^{n} k_i}$$

 k_i is, in our case, each of the arrows leading *away* from a given reservoir in Figure 22.6 of Seinfeld and Pandis. This formula yields the following lifetimes for each reservoir:

```
from IPython.display import Latex, display

reservoirs = {
    # name -> [amount (PgC), removal rate (PgC/yr)
    'M1': [612., 100. + 57. + 19],
    'M2': [730., 12. + 57. + 58.],
```

```
'M3': [140., 100. + 18.],
'M4': [37000., 40. + 70.],
'M5': [580., 50. + 50.],
'M6': [1500., 50.],
}

format_str = r"$\tau$(M$_{n:1d}$) = {tau:>5.1f} years"
for n in xrange(1, 7):
    [X, ks] = reservoirs['M%1d' % n]
    k = np.sum(ks)
    tau = X/ks
    display(Latex(format_str.format(n=int(n), tau=tau)))
```

$$\tau(M_1) = 3.5 \text{years}$$

 $\tau(M_2) = 5.7 \text{years}$
 $\tau(M_3) = 1.2 \text{years}$
 $\tau(M_4) = 336.4 \text{years}$
 $\tau(M_5) = 5.8 \text{years}$
 $\tau(M_6) = 30.0 \text{years}$

3.2 Problem 2

There are two different surface ocean reservoirs because the equilibrium dissolution of CO₂ in seawater is dependent on the water's temperature and pH.

CO₂ hydrolizes when it disolves in seawater:

$$\begin{aligned} \mathrm{CO_2(g)} + \mathrm{H_2O} & \Longrightarrow \mathrm{CO_2} \cdot \mathrm{H_2O} \\ \mathrm{CO_2} \cdot \mathrm{H_2O} & \Longrightarrow \mathrm{H^+} + \mathrm{HCO_3^-} \\ \mathrm{HCO_3^-} & \Longrightarrow \mathrm{H^+} + \mathrm{CO_3^{2--}} \end{aligned}$$

This produces both carbonate and bicarbonate ions. The abundance of dissolved salts in the ocean affects pH locally between a range of about 7.5 and 8.4, which is further impacted by temperature. Also, this reaction system is buffered; as CO_2 dissolves in seawater, that reservoir can take up less and less CO_2 from the atmosphere. The complexity of this reaction sequence is simplified in the compartmental model using a simple parameterization developed by Ver et al (1999), which modifies the loss mechanism of atmospheric CO_2 via dissolution in seawater as $F = kM^{\beta}$, where β is a positive constant which accounts for this complex chemistry. Using the two reservoirs and suitable associated β 's, the compartmental model can attempt to simulate oceanic carbon sink.

3.3 Problem 3

Assume that all the carbon in the atmosphere is present in the form of CO₂. The (volume) mixing ratio of a gas in the air is given as the ratio of a trace constituents molar concentration to that of the full gas. Note that this is a useful quantity to know because as the density of the air changes, the mixing ratio will remain the same, so one can always back out the mass of a given trace constituent with minimal extra information.

To a good approximation, the mean molecular weight of air can be computed just from the relative abundance and molecular weights of N:sub:2, CO₂, and Ar (which total 99.3% of the atmosphere by mass or volume):

$$M_a = (0.78 \cdot 28g/\text{mol}) + (0.21 \cdot 32g/\text{mol}) + (0.01 \cdot 40g/\text{mol}) \approx 28.97g/\text{mol}$$

(note that we rounded up the abundance of argon).

The molar mass of carbon is 12.01 g/mol; it's just about 16 g/mol for elemental oxygen, so carbon dioxide has a molar mass of 44.01 g/mol. If the pre-industrial atmospheric carbon burden was 612 Pg, then we can multiply by the molar ratio of carbon to carbon dioxide to yield the mass of CO₂ in the atmosphere,

$$\begin{aligned} \operatorname{Mass}(\operatorname{CO}_2) &= 612 \operatorname{Pg}(\operatorname{C}) \times \frac{44.01 \operatorname{g}(\operatorname{CO}_2)/\operatorname{mol}}{12.01 \operatorname{g}(\operatorname{C})/\operatorname{mol}} \\ &= 2244 \operatorname{Pg}(\operatorname{CO}_2) \end{aligned}$$

Since we know the mass of the atmosphere is roughly $5.15 \times 10^{18} \text{ kg}$, the mass mixing ratio of CO_2 is just

$$r(\text{CO}_2) = \frac{224.3 \text{Pg}}{5.15 \times 10^{18} \text{kg}} = 435.73 \text{ppm(m)}$$

To convert equivalently between mass mixing ratio and molar/volume mixing ratio, we have to account for difference in number concentrations of the molecules of each constituent, which are going to differ because they have molar mass. However, this computation can be radically shortened by noting that the mass mixing ratio is approximately equal to the molar mixing ratio times the ratio of the molar weight of the trace gas to the average molar weight of the entire gas,

$$\chi(\mathbf{X}) \frac{M(\mathbf{X})}{M_a} = \mathbf{r}(\mathbf{X})$$

Substituting in our intermediate values, we get

$$\chi(\text{CO}_2) = 435.73 \text{ppm(m)} \times \frac{28.97 \text{g/mol}}{44.01 \text{g/mol}} \approx 286.8 \text{ppm(v)}$$

which is a very reasonable estimate for pre-industrial CO₂ based on numerous proxy records.

3.3. Problem 3 15



NUMERICAL METHODS

I've implemented the model and integrators in Python (see the attached appendix). Note that I've wrapped the model using objects and classes to make my code easier to write and use - your mileage may vary on this front. But at the end of the day, your model should consist of two components:

- 1. An implementation of the right-hand side of the governing system of ODEs
- 2. An implementation of the integration/marching algorithm

The latter could be trivially simple. For instance, here is an implementation of the marching code using Euler's method:

```
def integrate(self, func, y0, t):
    out_y = [np.asarray(y0), ]

    for i, ti in enumerate(t[:-1]):
        y = out_y[-1]
        delta_t = t[i+1] - ti
        new_y = y + delta_t*func(y, ti)
        out_y.append(new_y)

return np.array(out_y)
```

The code merely evaluates the RHS equation (implemented by func) at each output instant and uses that to march forward in time.

I've written my code in a simple object-oriented framework, and attached it as appendices to this solution writeup. In the next cell, we execute the model code so that we can re-use it. In general, this sort of framework makes life a lot easier, because we can simply run the model with two or three lines of code, rather than have a messy for-loop and intermediate variable re-definition every single time we wish to run it.

First, let's look at the time-dependent emissions input, which we chose to be

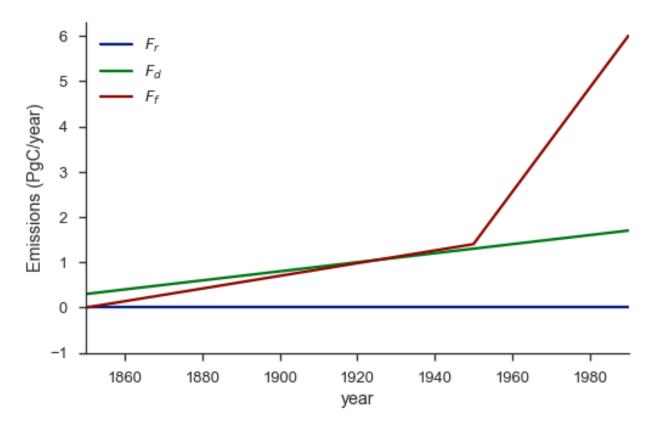
$$F_r(t) = 0$$

$$F_d(t) = 0.3 + 0.01t, (t = 0 \text{ for } 1850)$$

$$F_f(t) = \begin{cases} 0.014t & \text{from } 1850 \text{ to } 1950 \ (t = 0 \text{ for } 1850) \\ 1.4 + (4.6/40)t & \text{from } 1950 \text{ to } 1990 \ (t = 0 \text{ for } 1850) \end{cases}$$

This produces a time-varying emissions like,

```
t0, t_end = 1850, 1990
t = np.linspace(0, t_end - t0, t_end - t0 + 1)
## Vectorize the emissions function so we can quickly compute
## emissions for an array of times
emis vec = np.vectorize(emissions 22p6)
Fr, Fd, Ff = emis_vec(t)
with sns.color_palette("dark"):
   fig = plt.figure(figsize=(8,5))
    ax = fig.add_subplot(111)
    ax.plot(t+t0, Fr, label="$F_r$")
    ax.plot(t+t0, Fd, label="$F_d$")
    ax.plot(t+t0, Ff, label="$F_f$")
ax.set_ylim(-1)
ax.set_xlim(t0, t_end)
sns.despine()
ax.legend(loc='upper left')
ax.set xlabel("year")
ax.set_ylabel("Emissions (PgC/year)")
```



So clearly there is a big step up in fossil fuel emissions at 1950. We should think about this information when we evaluate our model's output - something should seriously change after 1950.

Reference the appendix for implementations of the solvers/marching algorithms. We'll go ahead and integrate the model using them all. Additionally, we'll use SciPy's `odeint http://docs.scipy.org/doc/scipy/reference/generated/scipy.integrate.odeint.html; __ wrapper as a reference solution. odeint wraps the industry standard LSODA algorithm via a package called ODEPACK - an old, Fortran-based library of ODE solvers. Specifically, LSODA uses a system's jacobian to more efficiently march forward in time within specified error and tolerance parameters. In cases where the user can define the time-dependent jacobian of a system they wish to solve, the method is particularly efficient - although it can approximate the jacobian with repeatd calls to the RHS if necessary. Furthermore, LSODA applies heuristics to the jacobian to analyze a system's stiffness, and can automatically switch between a stiff and non-stiff method based on where it can yield the most efficiency.

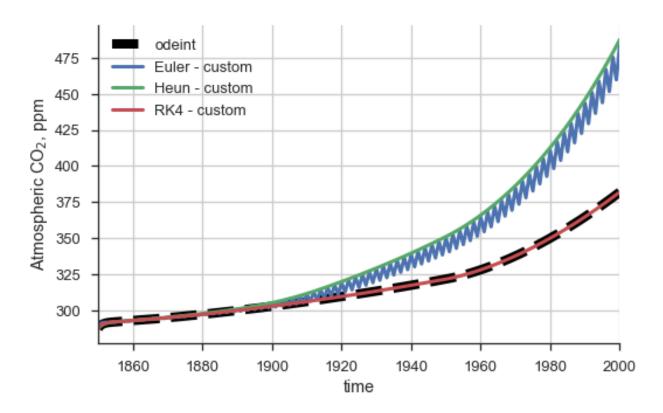
Below, we evaluate the model run with each of our numerical methods and the reference one. I'll annotate the code for the reference solution so it's clear what's happenening.

```
from scipy.integrate import odeint

# Record the initial conditions in an array
y0 = np.array([612, 730, 140, 37000, 580, 1500, 5300, 1.0])

# Define a custom emissions function. Here, we use one defined
```

```
# in the appending in carbon_model.py, and we over-ride its
# arguments such that the "switch" time when emissions turn on
# occurs 100 years into the simulation. We've assumed that the
# simulation will start at 1850, as per the documentation for the
# emissions function.
emis_func = lambda t: emissions_22p6(t, 100.)
# Instantiate the model. Note that we 'unpack' the initial condition
# array, to be consistent with the constructor for the model. We also
# explicitly pass the emissions function we just created.
model = CarbonModel(*y0, emis_func=emis_func)
# Some matplotlib commands to create a canvas for plotting.
fig = plt.figure(figsize=(8, 5))
ax = fig.add_subplot(111)
# Integrate the model using the `odeint` method, for 150. years.
output = model.integrate(odeint, 150.)
# Plot the output, setting some styles for its curve.
output['atm_ppm'].plot(ax=ax, style='--k', label="odeint",
                       lw=8)
plt.xlim(1850, 1959)
# We'll now repeat these steps using other numerical method interfaces.
with sns.color_palette("Paired"):
   print "Euler - custom"
   e = EulerIntegrator()
    o_eu_cust = model.integrate(e, 150., dt=1.)
    o_eu_cust.atm_ppm.plot(ax=ax, lw=3,
                           linestyle='solid', label="Euler - custom")
   print "Heun - custom"
   h = HeunIntegrator()
   o_eu_cust = model.integrate(h, 150., dt=1.)
   o_eu_cust.atm_ppm.plot(ax=ax, lw=3,
                           linestyle='solid', label="Heun - custom")
   print "RK4 - custom"
   r = RK4Integrator()
    o_rk4_cust = model.integrate(r, 150., dt=1.)
    o_rk4_cust.atm_ppm.plot(ax=ax, lw=3,
                            linestyle='solid', label="RK4 - custom")
ax.set ylabel("Atmospheric CO$ 2$, ppm")
plt.legend(loc='upper left')
plt.grid()
sns.despine()
```

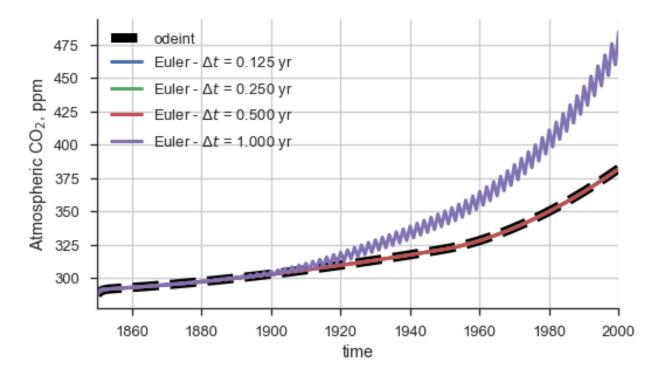


There are a few things to note on this plot.

First, only the Euler solution has an oscillating component in its projection of atmospheric CO₂ like we saw in the Mauna Loa data. However, is that a good thing? In this case, no - our model *shouldn't have that feature in its output*! If you inspect the model governing equations, you'll note that there is no component that should feature a seasonal signal. So this must be a deficiency in the solver. We might be able to eliminate it with a smaller timestep.

On the other hand, the RK4 solution at the same timestep converges to the reference solution. This is why it's important to know the limitations of your numerical methods and to have a good way to dial into a known solution!

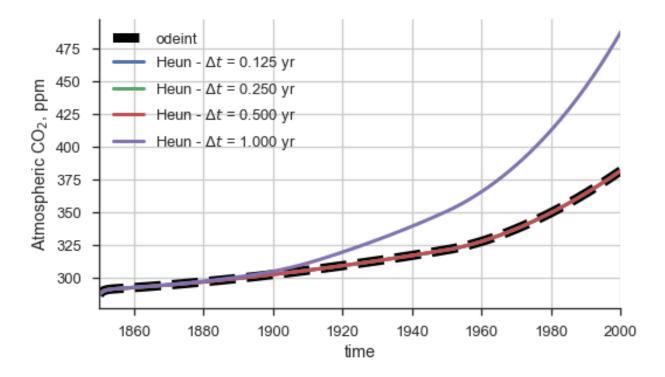
```
o = model.integrate(e, 150., dt=dt)
o.atm_ppm.plot(ax=ax, label=label, lw=3)
ax.set_ylabel("Atmospheric CO$_2$, ppm")
ax.legend(loc='upper left')
ax.grid()
sns.despine(fig)
```



That seems to be the case - even halving the timestep is enough to dramatically improve the solution.

Heun's Rule produces a similar issue, except without the oscillatory behavior. Reducing the timestep helps in that case, too:

```
o = model.integrate(h, 150., dt=dt)
o.atm_ppm.plot(ax=ax, label=label, lw=3)
ax.set_ylabel("Atmospheric CO$_2$, ppm")
ax.legend(loc='upper left')
ax.grid()
sns.despine(fig)
```



Let's use the RK4 implementation to find when CO2 doubles. We can naively do this by running our model for a longer period of time and inspecting the solution. Then, to get a numerical estimate, we can interpolate the model solution so that we have the atmospheric CO_2 as a smooth function of time. We can use simple root-finding methods like bisection or Newton-Raphson to then find the point where it doubles.

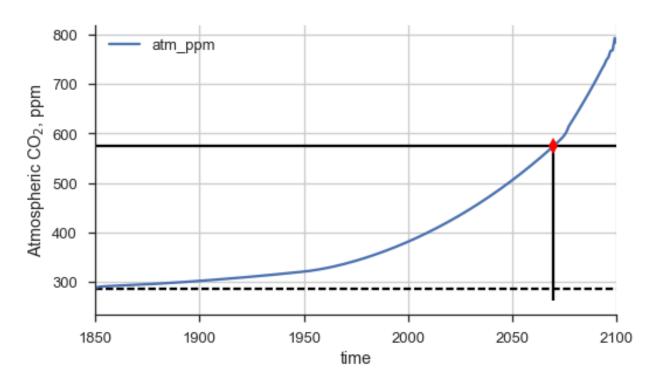
```
sns.set_palette("deep")
fig = plt.figure(figsize=(8, 10))
ax = fig.add_subplot(211)

plt.xlim(1850)

r = RK4Integrator()
o = model.integrate(r, 250., dt=dt)
o.atm_ppm.plot(ax=ax)

ax.set_ylabel("Atmospheric CO$_2$, ppm")
ax.legend(loc='upper left')
ax.grid()
```

```
CO2 doubles to 575 ppm in 2070
```



The CO₂ level doubles in 2070, so after about 180 years given the emissions scenario we used.

Alternatively, we could've implemented additional logic in our solver which would terminate the simulation once a specific ending condition was met (our doubling of CO_2 . In some cases, this is easy to do - for instance, some packages straightforwardly implement this into the integration routine logic they offer. Other times it may not be possible. Hence, the strategy we use here is

probably the best bet - run the model for a long time, interpolate the output, and then perform your analysis. This is going to be far more efficient than running the model many times!

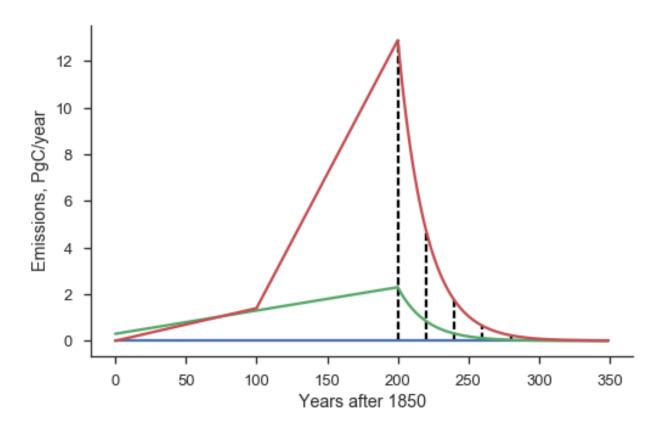
Suppose the world commits to decreasing its emissions in 2050. We'll model this scenario using an exponentially decaying emissions function which will kick in after some point. Assume the peak emissions occur in 2050 and save that value as F_{2050} (where all three components of the emissions are rolled into one vector). Then, we can write the emissions as

$$\mathbf{F}(t) = \mathbf{F}_{2050} \exp\left(-\frac{t - 2050}{\lambda}\right), \quad t > 2050$$

where λ is the e-folding constant, in years.

The easiest way to encode this emissions logic would be to wrap out original emissions function in a logical block which figures out which regime we're in. If it's before 2050, then it would spit back the original emissions values; if not, then it would return the time-decaying ones. We can write that function and visualize the emissions trace as a function of time:

```
def cust_emis(t, t_off=2050, t0=1850, lam=20.):
    """ t=0 corresponds to t0 """
    emis\_ref = emissions\_22p6(t)
    if t <= t_off - t0:
        return emis_ref
    else:
        E_2050 = np.array(emissions_22p6((t_off - t0)))
        # Swap the following lines to force the
        # de-forestation emissions to decay as well
        \#E_2050[2] = E_2050[2]*np.exp(-(t-(t_off - t0))/lam)
        E_2050 = E_2050*np.exp(-(t-(t_off - t0))/lam)
        return E_2050
lam = 20.
ts = np.arange(0., 2200-1850., 1.)
ee = np.array([cust_emis(ti, lam=lam) for ti in ts])
fig = plt.figure(figsize=(8,5))
ax = fig.add_subplot(111)
ax.plot(ts, ee)
ax.set_xlabel("Years after 1850")
ax.set_ylabel("Emissions, PgC/year")
for i in xrange(0, 6):
   x = (2050-1850) + i*lam
    ax.vlines(x, 0, cust\_emis(x, lam=lam)[-1],
              linestyles='dashed')
sns.despine(fig)
```



In this scenario, the emissions become negligible with 3 or 4 e-foldings (dashed lines in the reference plot). That's fine - does that mean that CO_2 will reduce on the same timescale of about 100 years?

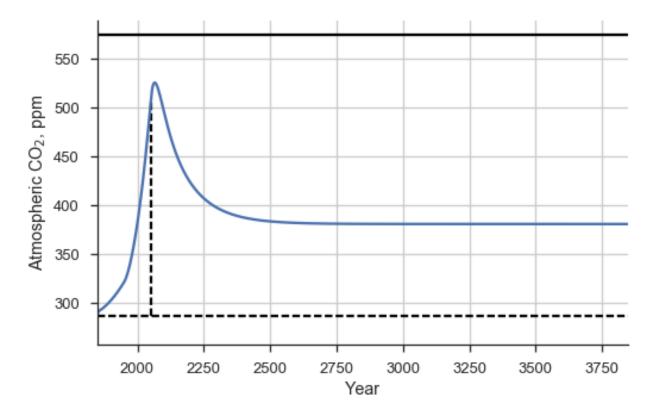
```
model = CarbonModel(*y0, emis_func=cust_emis)
r = RK4Integrator()
o = model.integrate(odeint, 2000., dt=0.25)
```

```
Doubling (initial) - 2069.64325981

Doubling (return) - 3214346871.43

Max - 525.899214083

Year Max - 2065.5
```



A few things are noteable about this graph.

1. Although the emissions begin to rapidly decay in 2050, the maximum atmospheric CO₂ (about 842 ppm) occurs two decades later in 2065).

Computational Methods Exercise - Solution, Release

- 2. To return to a state of doubled CO₂, it takes until 2229 or 162 years after the maximum CO₂ is observed, and just shy of 180 years after emissions begin to reduce!
- 3. We ran the simulation for 2000 years, and it did not return to pre-industrial levels. In fact, it plateaued at about 500 ppm, but not until after 2500 **700** years after the emissions began to ramp up.
- 4. Try running your simulation for 5000, 10000, or 50000 years (preferably with the reference numerical solver). In this model, the carbon sink from the atmosphere into all the other reservoirs is never enough to decrease the atmospheric CO₂ back to pre-industrial levels, regardless of how long you let the model run.

MODEL APPLICATION TO OBSERVED ATMOSPHERIC CO₂ CONCENTRATIONS

Finally, we'll apply our model to try to understand the 20th century atmospheric CO₂ record.

5.1 20th Century Emissions

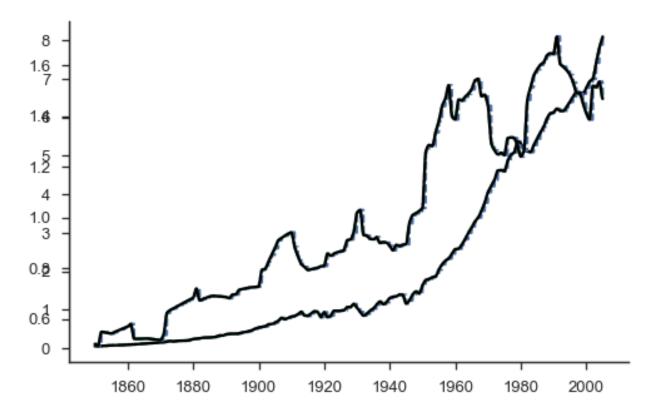
```
## Read in the data
# 1) Land-use data (TgC / year)
# in Excel spreadsheet form, should be fine w/ pandas
lu_data = pd.read_excel("Global_land-use_flux-1850_2005.xls",
                       sheetname="net fluxes", index_col=0)
# convert from TgC to PgC
lu_data = lu_data * 1e-3
#print lu_data.head()
# 2) Fossil-fuel data (million metric tons, which is one million
# megagrams or one teragram)
ff_data = pd.read_csv("global.1751_2010.csv", skiprows=[1,],
                     index col=0)
# convert to PgC
ff_{data} = ff_{data*1e-3}
#print ff_data.tail()
## 3) Collect into single dataframe
ff_col = 'Total carbon emissions from ' + \
         'fossil fuel consumption and ' + \
         'cement production (million ' + \
        'metric tons of C)'
ff_data.rename(columns={ff_col: 'fossil_fuel'}, inplace=True)
ff_series = ff_data['fossil_fuel']
lu_data.rename(columns={'Global': 'land_use'}, inplace=True)
lu_series = lu_data['land_use']
cdiac_data = pd.concat([lu_series, ff_series], axis=1)
## Some post-processing on the merged data
# a) interpolate linearly for any missing data
cdiac_data.interpolate(inplace=True)
# b) mask NaNs to 0
cdiac_data[np.isnan(cdiac_data)] = 0.
```

30

Interpolate the data using the various recommendations. We'll use PCHIP for the higher-order, piecewise-polynomial interpolation.

```
ts = np.linspace(1850, 2005, 12.*155 + 1.)
cx = cdiac_data.index.values
lu = cdiac_data['land_use'].values
ff = cdiac_data['fossil_fuel'].values
fig = plt.figure(figsize=(8, 5))
plt.clf()
ax_ff = fig.add_subplot(111)
ax_lu = plt.twinx(ax=ax_ff)
## Base data
#cdiac_data['land_use'].plot(ax=ax_lu, linewidth=5)
#cdiac_data['fossil_fuel'].plot(ax=ax_ff, linewidth=5)
#ax.set_xlim(1850, 2005)
## 1) Constant for each year
def emis_cdiac_floor(t):
   t_base = int(np.floor(t))
   idx = t base - cx[0]
   return 0., lu[idx], ff[idx]
yi = np.array([emis_cdiac_floor(t) for t in ts])
ax_lu.plot(ts, yi[:, 1], '--', label='LU - const')
ax_ff.plot(ts, yi[:, 2], '--', label='FF - const')
## 2) Linear interpolation
def emis_cdiac_linear(t):
    lu_int = np.interp(t, cx, lu)
    ff_int = np.interp(t, cx, ff)
    return 0., lu_int, ff_int
yi = np.array([emis_cdiac_linear(t) for t in ts])
ax_lu.plot(ts, yi[:, 1], '-.', label='LU - lin')
ax_ff.plot(ts, yi[:, 2], '-.', label='FF - lin')
## 3) PCHIP
from scipy.interpolate import PchipInterpolator
pchip_lu = PchipInterpolator(cx, lu)
pchip_ff = PchipInterpolator(cx, ff)
def emis_cdiac_pchip(t):
   return 0., pchip_lu(t), pchip_ff(t)
yi = np.array([emis_cdiac_pchip(t) for t in ts])
ax_lu.plot(ts, yi[:, 1], '-k', label='LU - pchip')
ax_ff.plot(ts, yi[:, 2], '-k', label='FF - pchip')
```

```
for i, x in enumerate([ax_lu, ax_ff]):
    ax.set_xlim(1980, 2000)
    ax.grid(False)
    if i == 1: ax.legend(loc='upper left')
sns.despine(fig)
```



Note - There's a caveat worth considering here with serious impacts when applying these techniques to true research. There are two ways to interpret the emissions data. On the one hand, we can simply view them as *intensities* or *instantaneous rates*. Under this interpretation, the interpolation techniques are valid in that we have a series of datapoints where an emissions intensity E was observed at some point in time t, and we wish to re-construct the time-depended function $\hat{E}(t)$ based on the dataset $\{(t_i, E_i)\}$.

But there's a different way to look at the data which might be more relevant. In that case, the emissions data is **not** instaneous. Rather, its an aggregate of how much was emitted over a given time period (in this case, a one year interval). Under this schema, we can't merely interpolate the emissions intensities as before. Instead, we need to interpolate with the condition that the integral of the emissions curve over the periods of time between observations is conserved. That is, our curve connecting January 1, 2014 to January 1, 2015 needs to conform to the fact that, say, 10 PgC was emitted in that same interval of time. Now we have an additional problem of *non-uniqueness*; you could possibly imagine that there are infinite families of interpolating factions that could satisfy these constraints.

With our linearly-interpolated emissions data, let's try to simulate the observed CO₂ record.

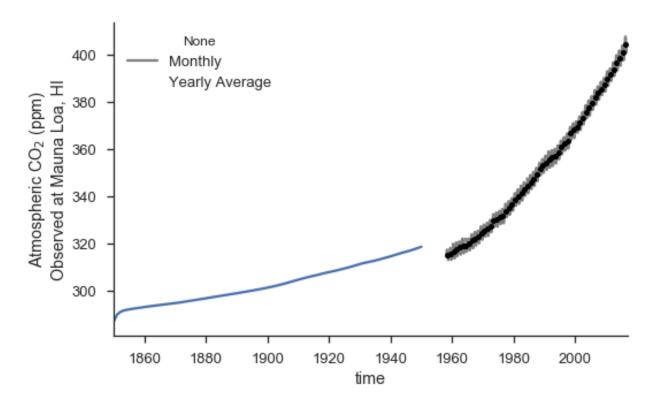
```
t_start = 1850
t_end = 1950
emis_wrap = lambda x: emis_cdiac_linear(t_start + x)

model = CarbonModel(*y0, emis_func=emis_wrap)
r = RK4Integrator()

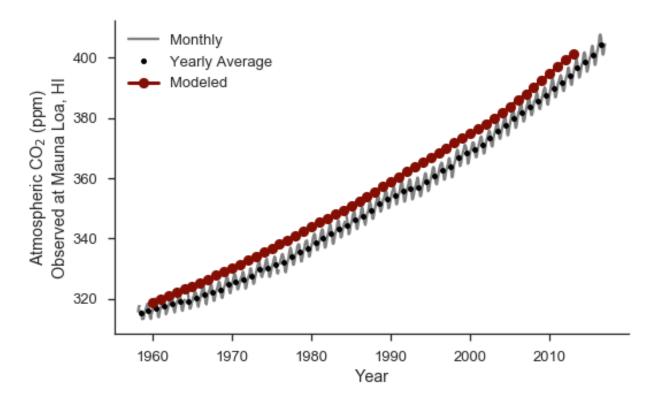
o_spinup = model.integrate(r, t_end - t_start, dt=1.)

fig = plt.figure(figsize=(8, 5))
ax = fig.add_subplot(111)
mauna_loa_plot(ax)
o_spinup.atm_ppm.plot(ax=ax)

y_1950 = o_spinup.iloc[-1].values[:-4]
```



Feed in the results from the simulation to 1950 as the initial conditions for a simulation running from 1960 to 2013.



That's not a bad fit at all! Accounting for our slight difference in initial conditions, we capture a reasonable rate of increase for atmospheric CO_2 , very much in line with the observational record. This is good evidence that our model does a reasonable job of reconciling the dynamics of the global carbon cycle - certainly well enough to dive deeper!

Repeat the previous exercise with the Global Carbon Budget dataset.

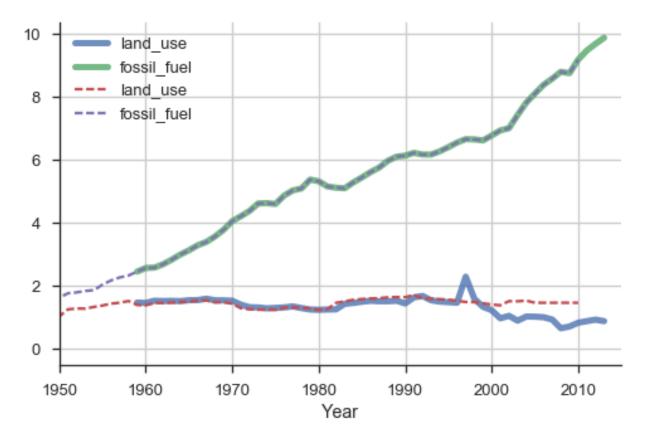
```
## Download the data
wget ftp://cdiac.ornl.gov/pub/Global_Carbon_Project/Global_Carbon_
→Budget_2014_v1.0.xlsx
```

```
--2017-01-30 14:42:14-- ftp://cdiac.ornl.gov/pub/Global_Carbon_
→Project/Global_Carbon_Budget_2014_v1.0.xlsx
          => 'Global_Carbon_Budget_2014_v1.0.xlsx.1'
Resolving cdiac.ornl.gov... 160.91.16.103
Connecting to cdiac.ornl.gov|160.91.16.103|:21... connected.
Logging in as anonymous ... Logged in!
==> SYST ... done. ==> PWD ... done.
==> TYPE I ... done. ==> CWD (1) /pub/Global_Carbon_Project ... done.
==> SIZE Global_Carbon_Budget_2014_v1.0.xlsx ... 512344
==> PASV ... done. ==> RETR Global_Carbon_Budget_2014_v1.0.xlsx ...

done.
Length: 512344 (500K) (unauthoritative)
\rightarrowin 0.3s
2017-01-30 14:42:15 (1.48 MB/s) - 'Global_Carbon_Budget_2014_v1.0.xlsx.
\rightarrow1' saved [512344]
```

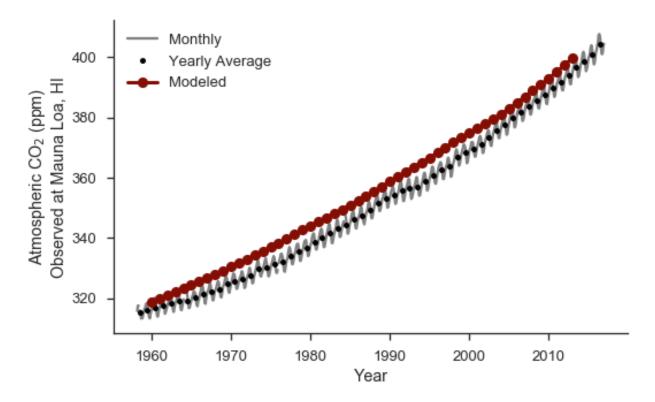
For quick reference, let's plot the GCB emissions data against the CDIAC emissions data:

```
ax.set_xlim(1950, 2015)
ax.grid()
sns.despine()
```



There's not much of a difference, except the GCB data (in the solid colors) seems to capture a bit more nuance in the land-use budget after 1995.

Using the Global Carbon Budget as our emissions, let's re-run the compartmental model from the branch-off point we previously used with CDIAC:



Once again, we very closely reproduce the observed record from Mauna Loa. In fact, we tend to improve the simulation post 1995 - we capture the rate of increase a bit more exactly, although in actuality we made only a modest tweak to the total emissions.

5.2 Looking Towards the Future

Now that we have some confidence in our model's ability to capture reality, let's apply it to understand something about future climate change. To do this, we'll use the "Representative Concentration Pathways" (RCP) which were previously used in the CMIP5 global climate model intercomparison. These RCPs are hypothetical scenarios describing how future greenhouse gas emissions might change. In a climate model, we'd use them as input to determine the atmospheric concentration in each year for use with the model's radiation module (with a caveat - some models have a global interactive carbon cycle, so in that case you'd use a slightly different formulation, but with

the advantage of detecting feedbacks from that system).

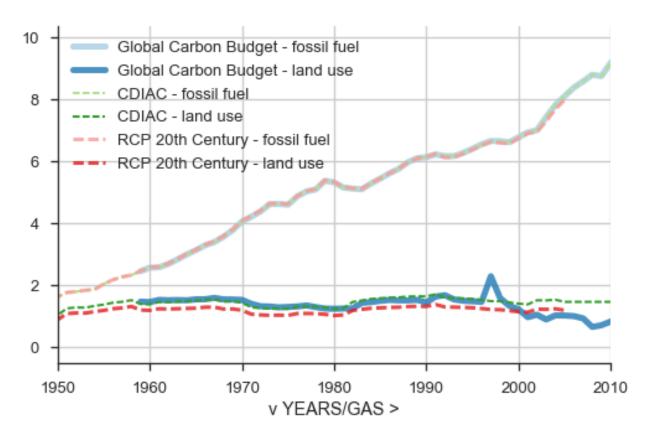
For our purposes, let's just simulate how the emissions scenarios would matriculate into future CO_2 concentrations. We'll start by reading in the emissions scenarios and plotting them as before.

```
## Download the CMIP5 data
wget http://www.pik-potsdam.de/~mmalte/rcps/data/20THCENTURY_EMISSIONS.

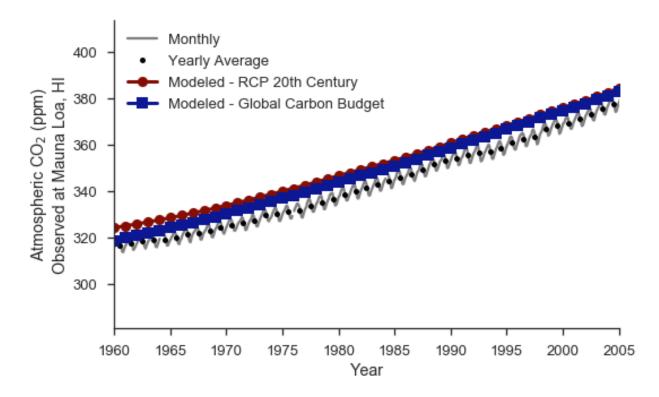
-xls
wget http://www.pik-potsdam.de/~mmalte/rcps/data/RCP3PD_EMISSIONS.xls
wget http://www.pik-potsdam.de/~mmalte/rcps/data/RCP45_EMISSIONS.xls
wget http://www.pik-potsdam.de/~mmalte/rcps/data/RCP6_EMISSIONS.xls
wget http://www.pik-potsdam.de/~mmalte/rcps/data/RCP6_EMISSIONS.xls
wget http://www.pik-potsdam.de/~mmalte/rcps/data/RCP85_EMISSIONS.xls
```

```
## Read in the 20th century emissions database, construct
## time-varying emissions function, and produce a simulation of
## the 20th century
rcp_20th = pd.read_excel("20THCENTURY_EMISSIONS.xls",
                         sheetname="20THCENTURY_EMISSIONS",
                         skiprows=36, index_col=0)
index_map = {"v YEARS/GAS >": "years", }
col_map = {"FossilCO2": "fossil_fuel", "OtherCO2": "land_use"}
rcp_20th.rename(index_map, col_map, inplace=True)
cx = rcp_20th.index.values
lu = rcp_20th['land_use'].values
ff = rcp_20th['fossil_fuel'].values
def emis_rcp_20th_linear(t):
    lu_int = np.interp(t, cx, lu)
    ff_int = np.interp(t, cx, ff)
   return 0., lu_int, ff_int
split_str = lambda s : s.replace("_", " ")
with sns.color_palette('Paired'):
   fig = plt.figure(figsize=(8, 5))
    ax = fig.add_subplot(111)
    for name, df, ls, lw, alpha in \
        [('Global Carbon Budget', gcb, 'solid', 5., 0.8),
         ('CDIAC', cdiac_data, '--', 2., 1.0),
         ('RCP 20th Century', rcp_20th, '--', 3., 0.8)]:
        for key in ["fossil_fuel", "land_use"]:
            df[key].plot(ax=ax, lw=lw, ls=ls, alpha=alpha,
                         label="%s - %s" % (name, split_str(key)))
    ax.legend(loc='upper left')
    ax.grid()
```

```
ax.set_xlim(1950, 2010)
sns.despine()
```



We notice that 20th Century RCP analysis slightly disagrees with both the CDIAC and GCB ones. However, the difference is enough that we might be interested in how this affects our simulation of 20th century atmospheric carbon dioxide, so we should plot up a quick comparison.



Actually, not much of a difference.

5.3 Projection of future climate change using RCP scenarios

Now, let's simulate the future climate change scenarios defined by each RCP. This cell will combine everything we've done so far: loading in an emissions dataset, converting it to a function,

instantiating a model run, and running the model.

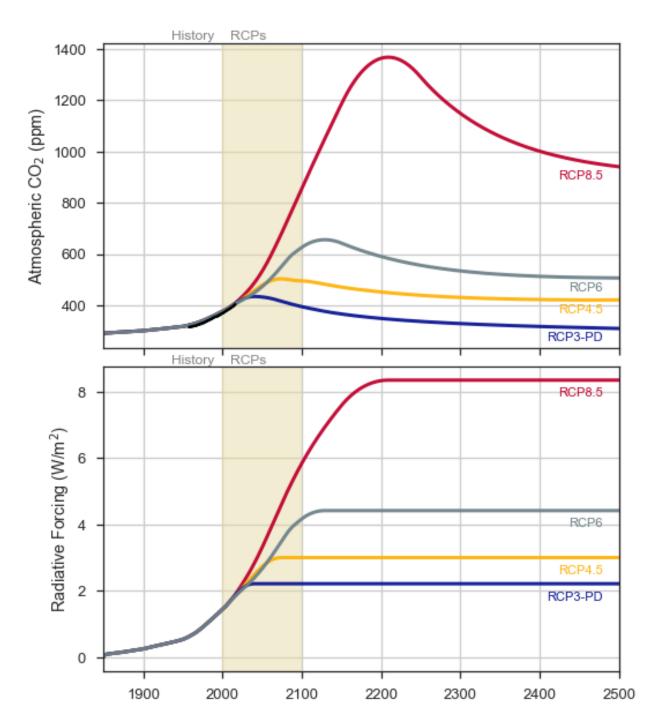
```
scenarios = {
   "RCP3-PD": {
        'short': "RCP3PD",
        "description": "Low RCP with pick and decline",
        "color": sns.xkcd_rgb['royal'],
    } ,
    "RCP4.5": {
        'short': "RCP45",
        "description": "Medium-low RCP with stabilisation from 2150...

→onwards",
        "color": sns.xkcd_rgb['amber'],
    },
    "RCP6": {
        'short': "RCP6",
        "description": "Medium-high RCP with stabilisation from 2150...
        "color": sns.xkcd_rqb['steel grey'],
    },
    "RCP8.5": {
        'short': "RCP85",
        "description": "High RCP, stabilising emissions post-2100,...
→concentrations post-2200",
        "color": sns.xkcd rqb['lipstick red'],
   },
}
for rcp in scenarios.keys():
   print rcp, scenarios[rcp]['description']
    ## Read emissions
    short = scenarios[rcp]['short']
    rcp_emis = pd.read_excel("%s_EMISSIONS.xls" % short,
                             sheetname="%s_EMISSIONS" % short,
                             skiprows=37, index_col=0)
    index_map = {"v YEARS/GAS >": "years", }
    col_map = {"FossilCO2": "fossil_fuel", "OtherCO2": "land_use"}
    rcp_emis.rename(index_map, col_map, inplace=True)
    scenarios[rcp]['emissions'] = rcp emis
    ## Linearly interpolate emissions
    cx = rcp emis.index.values
    lu = rcp_emis['land_use'].values
    ff = rcp_emis['fossil_fuel'].values
    def emis_rcp_linear(t):
```

Plot the results, adding some useful details to the figure.

42

```
fig, [ax_C02, ax_RF] = plt.subplots(2, 1, figsize=(8, 10),
                                    sharex=True)
plt.subplots_adjust(hspace=0.06)
for rcp in scenarios.keys():
   output = scenarios[rcp]['output']
   color = scenarios[rcp]['color']
   output.atm_ppm.plot(ax=ax_CO2, color=color,
                        lw=3, alpha=0.95, label=rcp)
    ax_CO2.text(2480, output.atm_ppm.ix[2500]-50., rcp,
            color=color, ha='right', size=11)
   mauna_loa_yearly.average.plot(ax=ax_CO2, color='k')
    delta_F = 5.35*np.log(output.atm_ppm/output.atm_ppm.ix[1850])
    idx_max = np.argmax(delta_F)
    delta F.ix[idx max:] = delta F.ix[idx max]
    delta_F.plot(ax=ax_RF, color=color, lw=3, alpha=0.95,
                 label=rcp)
    ax_RF.text(2480, delta_F.ix[2500]-0.5, rcp,
```



This plot is similar to what's on the RCP website. For simplicity, I froze the radiative forcing plots at their maximum values.

There are many clear implications of these simulations. For starters, the high-emissions scenario produce a significant amount of radiative forcing up to and beyond the year 2100. This would have substantial impacts on our global climate - including significant warming in the global average. The radiative equivalent of doubling CO₂ is about 4 degrees per watt per meter-squared. For a rough and dirty calculation, in the RCP8.5 case, this would yield a little more than 6 degrees of warming in equilibrium. That's *a lot*!

Of course, this neglects many things. For instance, what might happen to the carbon cycle in a warming climate? Consider the land-use budget we use in our emissions. Although de-forestation is a major component of it, shifts in precipitation and temperature could also affect the type and presence of vegetation in many places around the world. If precipitation were to drastically decrease in a region that otherwise would experience a large amount on average, significant loss of vegetation could occur and affect the magnitude of the global carbon sink. In that sense, there would be a *positive feedback* on climate change - the shrinking of the carbon sink as the world warms would, on average, tend to increase the rate of increase of carbon in the atmosphere, producing even more warming. Constraining the magnitude of global carbon cycle feedbacks is a major contemporary research issue, and some modern global models even include detailed carbon cycle models (much more so than what we've done here - real models coupled to the chemistry and biology of the oceans and land surface) to reconcile these effects.

Computational Methods Exercise	- Solution, Release

CHAPTER

SIX

CODE SAMPLES

The following listings contain reference implementations of the modular compartmental carbon cycle model I developed to solve this exercise. You're encouraged to refine them and fine-tune them to your own needs.

6.1 Compartmental Carbon Cycle Model

Listing 6.1: carbon_model.py - An implementation of the compartmental carbon model using a flexible interface for time integration.

```
""" Implementation of Compartmental of Carbon Cycle model.
  Author: Daniel Rothenberg <darothen@mit.edu>
   Version: February 13, 2015
   m m m
6
  import numpy as np
  import pandas as pd
10
   class CarbonModel (object):
11
       """ Container class implementing Compartmental Carbon Cycle
12
       model.
13
14
       This class encapsulates the logic for instantiating, integrating,
15
       and analyzing a multi-component model of the carbon cycle. It is
       designed to simplify the task of repeateadly running the model
17
       with different parameters - including emissions functions - and
18
       for saving and storing the results. Running the model is very,
19
   ⇔simple:
20
       11 11 11
21
```

```
## Default Parameters
23
24
       beta_2 = 9.4
25
       beta_3 = 10.2
26
       gamma = 62.0
27
       Gamma = 198.
28
       a_d = 0.230
29
       a_r = 1.0
30
31
       k_12 = 0.0931
32
       k_13
             = 0.0311
33
       k_15
               = 147.0
34
       k 21
              = 58.*(720.**(-beta_2))
35
       k_23
               = 0.0781
36
       k 24
             = 0.0164
37
       k_31
               = 18.*(140.**(-beta_3))
38
       k_34 = 0.714
39
       k_42 = 0.00189
40
       k_43
             = 0.00114
41
       k_{51} = 0.0862
42
       k_56
               = 0.0862
43
       k_61
             = 0.0333
44
45
       def __init__(self, M1, M2, M3, M4, M5, M6, M7, G, emis_func,
46
                      **kwargs):
47
48
            ## Initial Conditions
49
            self.M1 = M1
50
           self.M2 = M2
51
           self.M3 = M3
52
           self.M4 = M4
53
           self.M5 = M5
54
           self.M6 = M6
55
           self.M7 = M7
56
           self.G = G
57
58
           self.emis_func = emis_func
59
60
           self.y0 = [M1, M2, M3, M4, M5, M6, M7, G]
61
62
            for key, value in kwargs.iteritems():
63
                self.__dict__[key] = value
64
65
       def __call__(self, y, t):
66
            """ Alias to call the ``rhs'' method.
67
68
            n n n
69
```

```
return self.rhs(y, t)
70
71
        def rhs(self, y, t):
72
            """ Evaluate the RHS of the model governing equations
73
74
            n n n
75
76
            M1, M2, M3, M4, M5, M6, M7, G = y[:]
77
            F_r, F_d, F_f = self.emis_func(t)
78
79
            dM1_dt = -1.*(self.k_12 + self.k_13)*M1 \setminus
                    - self.k_15*G*(M1 - self.gamma)/(M1 + self.Gamma) \setminus
81
                    + self.k 21*(M2**self.beta 2) + self.k 31*(M3**self.
82
    →beta_3) \
                    + self.k 51*M5 \
83
                    + self.k_61*M6 + F_f + F_d - F_r
84
            dM2 dt = self.k 12*M1 \setminus
85
                    - (self.k_23 + self.k_24)*M2 - self.k_21*(M2**self.beta_
    →2) \
                    + self.k_42*M4
87
            dM3_dt = self.k_13*M1 + self.k_23*M2 - self.k_34*M3 \setminus
88
                    - self.k_31*(M3**self.beta_3) \
89
                    + self.k_43*M4
90
            dM4_dt = self.k_24*M2 + self.k_34*M3 - (self.k_42 + self.k_
91
    \hookrightarrow 43) \star M4
            dM5_dt = self.k_15*G*(M1 - self.gamma)/(M1 + self.Gamma) \setminus
                    - (self.k_51 + self.k_56) \starM5 \
93
                    - F d + F r
94
            dM6 dt = self.k 56*M5 - self.k 61*M6
95
            dM7 dt = -1.*F f
96
            dG_dt = -1.*(self.a_d*F_d - self.a_r*F_r)/self.M5 # note that_
97
    ⇒self.M5 is
                                                                      # frozen to
    →the initial
                                                                      # M5
99
100
            dy_dt = [dM1_dt, dM2_dt, dM3_dt, dM4_dt, dM5_dt, dM6_dt,
101
                        dM7_dt, dG_dt ]
102
103
            return np.array(dy_dt)
104
        def _output(self, t, u, t_offset):
106
            """ Process the model output into a descriptive DataFrame
107
108
            M cols = ["M%1d" % i for i in range(1, 8)]
109
            tt = pd.Series(t, name="time") + t_offset
110
            yy = pd.DataFrame(u,
111
```

```
columns=M_cols + ["G", ],
112
                                 index=tt)
113
114
            ppm_fac = 1./2.13 \#: ppmv / PgC
115
116
            yy['atm_ppm'] = yy.M1*ppm_fac
117
118
            yy_emis = pd.DataFrame([self.emis_func(ti) for ti in tt],
119
                                      columns=["F_r", "F_d", "F_f"],
120
                                      index=tt)
121
122
            yy = pd.concat([yy, yy_emis], axis=1)
123
124
            return yy
125
126
        def integrate(self, integrator, t_end, dt=1./365.,
127
                       t_offset=1850., ):
128
             """ Interface for integrating the model using custom
129
            integration schemes.
130
             m m m
131
132
            t = np.arange(0., t_end+dt, dt)
133
            y = integrator(self, self.y0, t)
134
135
            return self._output(t, y, t_offset)
136
137
        def integrate_odespy(self, integrator, t_end, dt=1./365.,
138
                               t offset=1850.):
139
             """ Interface for running the model using integration
140
            schemes from odespy package
141
            11 11 11
142
143
            t = np.arange(0., t\_end+dt, dt)
144
            solver = integrator(self)
145
            solver.set_initial_condition(self.y0)
146
            y, t = solver.solve(t)
147
148
            return self._output(t, y, t_offset)
149
150
    ## Boundary conditions
151
   def emissions_22p6(t, switch=100.):
152
        """ Return 3 values, corresponding to fluxes F_r, F_d, and F_f
153
        evaluated at a given time 't'
154
155
        Fluxes are in Pg(C)/yr; time 't' is in years since
156
        a particular baseline (1850 in this case)
157
158
```

```
F_r = 0.

F_d = 0.3 + 0.01*t

F_f = 0.014*t if t <= switch else 1.4 + (4.6/40.)*(t - 100.)

return F_r, F_d, F_f
```

6.2 Modular Integrator Abstract Class

Listing 6.2: integrator.py - A modular time-integration scheme for ODEs

```
""" Implementation of numerical integration schemes.
  Author: Daniel Rothenberg <darothen@mit.edu>
   Version: February 13, 2015
   m m m
6
  import abc
  import numpy as np
10
  class Integrator:
11
       """ This is an abstract class providing a template for
12
       integration routine logic.
13
14
       All integration routines need to implement an `integrate`
15
       method, which march a system of ODEs forward in time over
16
       discrete timesteps from some initial conditions, given a
17
       function which implements the RHS of that ODE system.
18
19
       n n n
20
21
       __metaclass__ = abc.ABCMeta
22
23
       @staticmethod
24
       @abc.abstractmethod
       def integrate(self, func, y0, t):
           """Performs the integration"""
27
28
       def __call__(self, func, y0, t):
29
           return self.integrate(func, y0, t)
30
31
  class EulerIntegrator(Integrator):
33
       def integrate(self, func, y0, t):
```

```
out_y = [np.asarray(y0),]
35
           for i, ti in enumerate(t[:-1]):
36
                y = out_y[-1]
37
                delta_t = t[i+1] - ti
38
                new_y = y + delta_t * func(y, ti)
39
                out_y.append(new_y)
40
           return np.array(out_y)
41
42
   class HeunIntegrator(Integrator):
43
44
       def integrate(self, func, y0, t):
           out_y = [np.asarray(y0), ]
46
           for i, ti in enumerate(t[:-1]):
47
                y = out_y[-1]
48
                delta_t = t[i+1] - ti
49
50
                y_tilde = y + delta_t*func(y, ti)
51
                new_y = y + \setminus
52
                    (delta_t/2.)*(func(y, ti)
53
                                    + func(y_tilde, ti+delta_t) )
54
                out_y.append(new_y)
55
           return np.array(out_y)
56
57
   class RK4Integrator(Integrator):
58
59
       def integrate(self, func, y0, t):
60
           out_y = [np.asarray(y0),]
61
            for i, ti in enumerate(t[:-1]):
62
                y = out_y[-1]
63
                delta_t = t[i+1] - ti
64
65
                k1 = func(y, ti)
66
                k2 = func(y + 0.5*k1*delta_t, ti + 0.5*delta_t)
                k3 = func(y + 0.5*k2*delta_t, ti + 0.5*delta_t)
68
                k4 = func(y + k3*delta_t, ti + delta_t)
69
70
                new_y = y + (delta_t/6.) * (k1 + 2.*k2 + 2.*k3 + k4)
71
                out_y.append(new_y)
72
           return np.array(out_y)
73
```