Kppa Verification using KPP-generated code

```
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```

Description

Shows results from `small` as generated by KPP and Kppa. The Kppa code has been modified to match KPP's integration limits, use Rodas3, use KPP's sunlight approximation, and use a constant temperature of 270K.

Instructions

1. Compile and run the `small` and `small_kpp221` codes
2. Execute all cells in this notebook.

In [136]:
```
kppa_file = 'small/small.dat'
kpp_file = 'small_kpp221/small_f90.dat'
```

Processing Script

Skip down for results

In [137]:
```
%matplotlib inline
import re
from itertools import cycle
from pylab import *
from matplotlib.markers import MarkerStyle
import matplotlib.pyplot as plt

ATOL = 1.0e-3
RTOL = 1.0e-4
EPS = 2.2204460492503131E-016
REGEX = re.compile('^([+\-]?)([0-9.]+)e?([+\-])([0-9.]+)$')
def convert(s):
    """
    Converts a number in Fortran E24.16 format to a Python float
    """
    m = re.search(REGEX, s)
    if m:
        s = ''.join([m.group(1), m.group(2), 'e', m.group(3), m.group(4)])
    try:
        fval = float(s)
    except ValueError:
        print '================> %s' % s
        fval = 0.0
    if fval < EPS:
```

```
        return 0.0
    else:
        return fval

def read_datfile(fname, tstart, cstart):
    """
    Read data from fname beginning on line tstart with concentration data be
ginning in field cstart.
    Returns a tuple: (time, concentrations)
    Time data:
        [t0 t1 ... tN]
    Concentration data:
        [ [SPC_0(t0) SPC_1(t0) ... SPC_N(t0)]
          [SPC_0(t1) SPC_1(t1) ... SPC_N(t1)]
              :         :             :
          [SPC_0(tN) SPC_1(tN) ... SPC_N(tN)] ]
    """
    t = []
    c = []
    with open(fname, 'r') as f:
        while tstart:
            f.readline()
            tstart -= 1
        for line in f:
            parts = line.split()
            t.append(convert(parts[0]))
            c.append([convert(x) for x in parts[cstart:]])
    return t, c

def plot_dat(data, xlabel='Time', ylabel='Conc', names=None, titles=None):
    """
    Draw a plot of data read from read_datfile
    """
    lines = ['-', '--', '-.', ':']
    markers = MarkerStyle.filled_markers
    linecycler = cycle(lines)
    markercycler = cycle(markers)
    datastyles = ['%s%s' % (linecycler.next(), markercycler.next()) for _ in
 data]
    ndat = len(data)
    nspec = len(data[0][1][0])
    x = data[0][0]
    for i in xrange(0, nspec):
        fig, ax = plt.subplots()
        for j, dat in enumerate(data):
            t, c = dat
            y = [ct[i] for ct in c]
            style = datastyles[j]
            if names:
                label = '%s' % names[j]
            else:
                label = '%d' % j
            ax.plot(x, y, style, label=label)
        if ndat > 1:
            ax.legend(loc=2)
        ax.set_xlabel(xlabel)
```

```
        ax.set_ylabel(ylabel)
        if titles:
            ax.set_title(titles[i])
        else:
            ax.set_title('Species %d' % i)
        show()

def scaled_err(x, y):
    if x or y:
        return abs(x-y)/max(x, y)
    elif x == y:
        return 0.0
    else:
        return float('inf')

def calc_err(d0, d1):
    c0 = d0[1]
    c1 = d1[1]
    err = []
    nsteps = len(c0)
    nspec = len(c0[0])
    sigPow = 0.0
    errPow = 0.0
    errCount = 0.0
    for i in xrange(0, nsteps):
        e = []
        for j in xrange(0, nspec):
            x = c0[i][j]
            y = c1[i][j]
            sigPow += x*x
            errPow += (x-y)*(x-y)
            serr = scaled_err(x,y)
            if serr > RTOL:
                print '%g > %g: %g, %g' % (serr, RTOL, x, y)
                errCount += 1
            e.append(serr)
        err.append(e)
    if errPow > 0:
        snr = 20 * log10(sigPow / errPow)
    else:
        snr = float('inf')
    print 'SNR: %fdb' % snr
    if errCount:
        print '%d samples with relative error > %g' % (errCount, RTOL)
    return d1[0], err
```

In [138]:
```
kppa_dat = read_datfile(kppa_file, 0, 3)
kpp_dat = read_datfile(kpp_file, 1, 1)
```

Results: Relative Error and SNR

The following cell shows the relative error per concentration for each time step written to the `.dat` files. A signal-to-noise ratio and relative error count are shown below. As a rule of thumb, SNR >= 250 indicates solution match to five decimal places. This is a **relative error calculation**, so concentrations close to zero are likely to have high relative error but low absolute error.

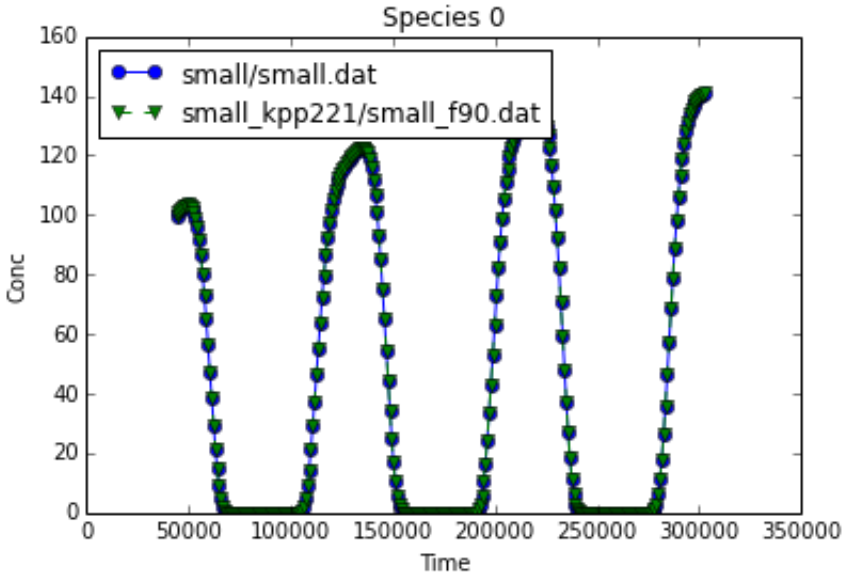
In [139]:
```
err_dat = calc_err(kpp_dat, kppa_dat)
```

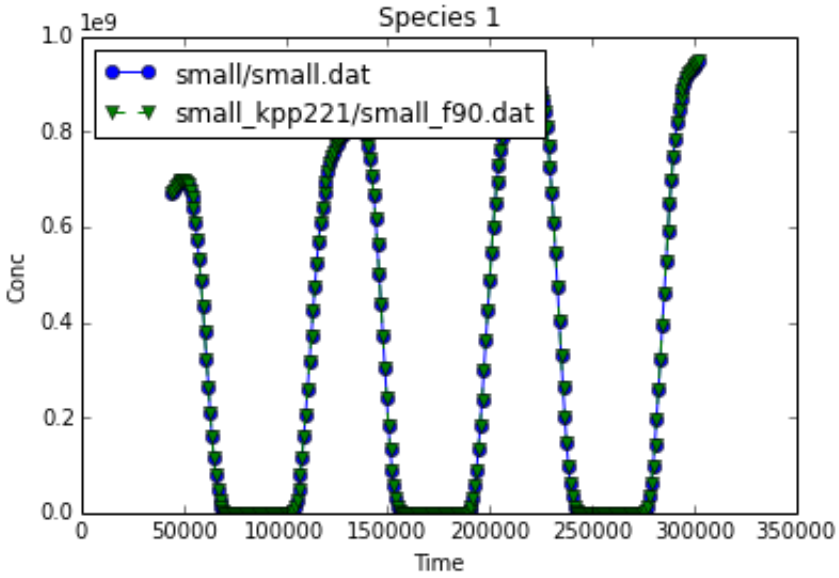
```
0.000152216 > 0.0001: 2.26933e+08, 2.26898e+08
0.000441163 > 0.0001: 0.0349329, 0.0349484
0.110534 > 0.0001: 0.00123054, 0.00109453
0.113944 > 0.0001: 3.31012e-05, 2.93295e-05
1 > 0.0001: 8.90411e-07, 0
0.0623772 > 0.0001: 2.39518e-08, 2.55452e-08
1 > 0.0001: 6.44294e-10, 0
0.221036 > 0.0001: 1.73313e-11, 2.22492e-11
1 > 0.0001: 4.66206e-13, 0
0.352848 > 0.0001: 1.25408e-14, 1.93784e-14
1 > 0.0001: 3.37343e-16, 0
0.000385351 > 0.0001: 0.0523142, 0.0523344
0.151055 > 0.0001: 0.000938435, 0.00110541
1 > 0.0001: 9.66625e-06, 0
0.97291 > 0.0001: 9.95662e-08, 3.67539e-06
1 > 0.0001: 1.02557e-09, 0
0.999136 > 0.0001: 1.05638e-11, 1.22203e-08
1 > 0.0001: 1.08811e-13, 0
0.999972 > 0.0001: 1.1208e-15, 4.06312e-11
1 > 0.0001: 0, 1.35094e-13
1 > 0.0001: 0, 4.49175e-16
0.000315788 > 0.0001: 0.00847613, 0.00847881
0.606772 > 0.0001: 9.10626e-05, 3.58083e-05
1 > 0.0001: 3.11266e-07, 0
0.935 > 0.0001: 1.06396e-09, 1.63686e-08
1 > 0.0001: 3.63677e-12, 0
0.99985 > 0.0001: 1.24311e-14, 8.29714e-11
1 > 0.0001: 0, 4.20576e-13
1 > 0.0001: 0, 2.13187e-15
SNR: 421.844511db
29 samples with relative error > 0.0001
```

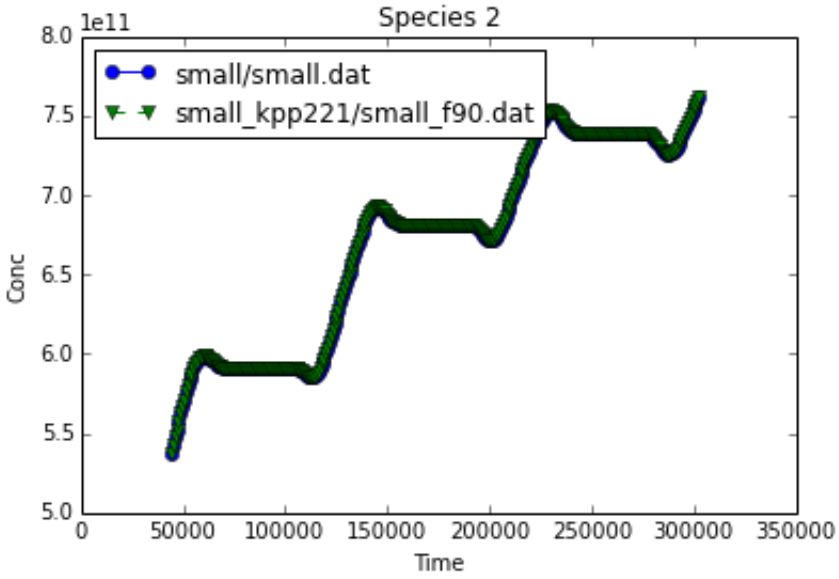
Results: Concentration vs. Time

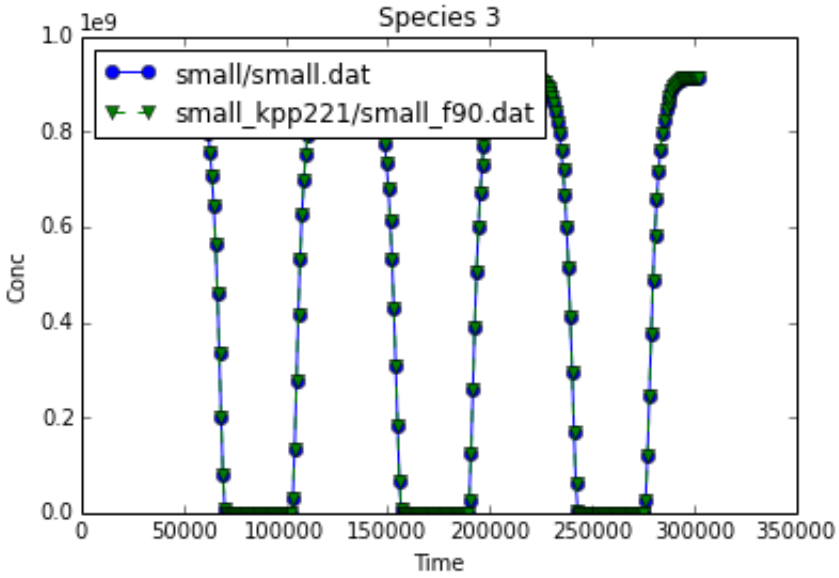
The following charts show concentrations from both files vs. time. The species name is not recored in the `.dat` file, but you can replace `None` in the `plot_dat` call with an ordered list of names to set the plot titles.

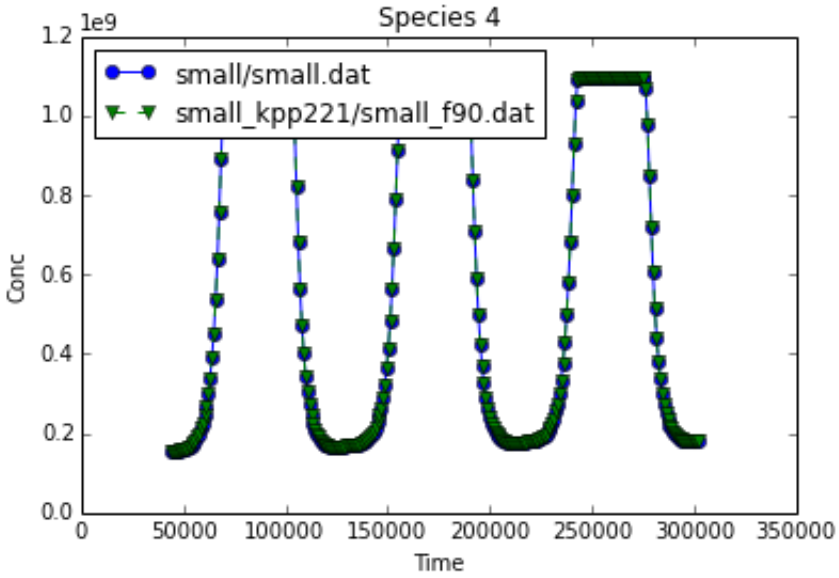
In [140]:
```
plot_dat([kppa_dat, kpp_dat], names=[kppa_file, kpp_file], titles=None)
```

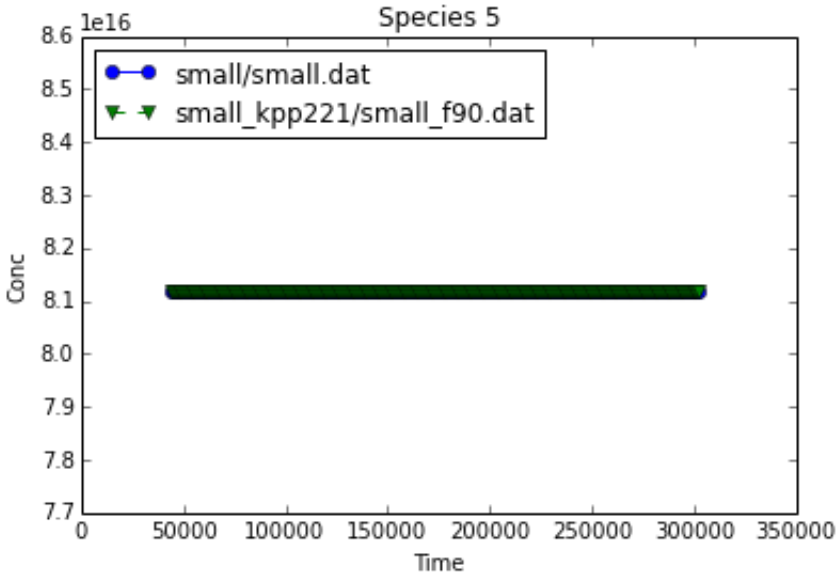

Species 0
small/small.dat
small_kpp221/small_f90.dat
Conc
Time
0
20
40
60
80
100
120
140
160
0
50000
100000
150000
200000
250000
300000
350000

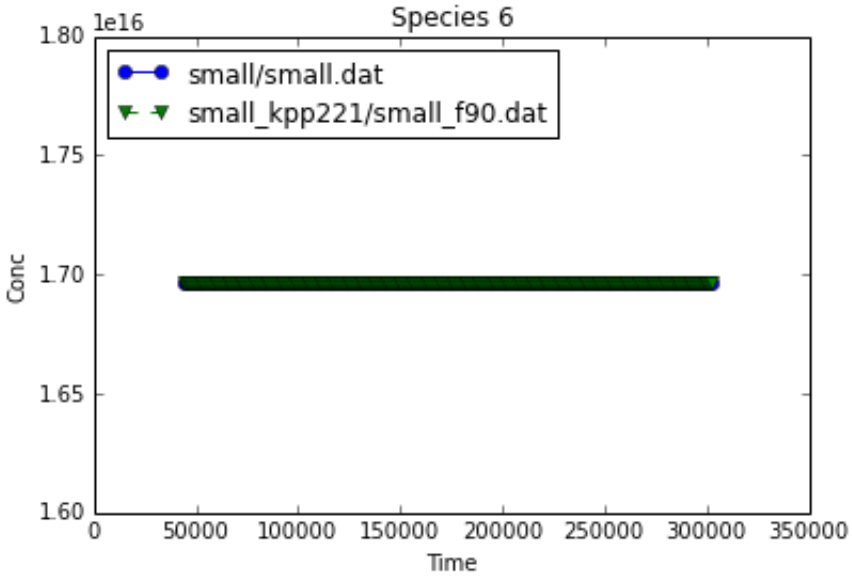

Species 1
1e9
small/small.dat
small_kpp221/small_f90.dat
Conc
Time
0.0
0.2
0.4
0.6
0.8
1.0
0
50000
100000
150000
200000
250000
300000
350000


Species 2
1e11
small/small.dat
small_kpp221/small_f90.dat
Conc
Time
5.0
5.5
6.0
6.5
7.0
7.5
8.0
0
50000
100000
150000
200000
250000
300000
350000


Species 3
1e9
small/small.dat
small_kpp221/small_f90.dat
Conc
Time


Species 4
1e9
small/small.dat
small_kpp221/small_f90.dat
Conc
Time

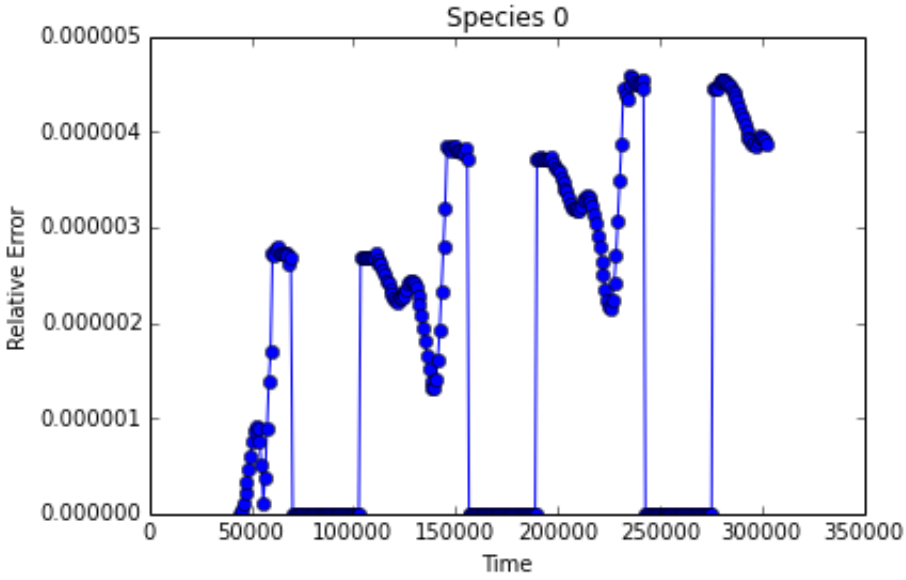

Species 5
1e16
small/small.dat
small_kpp221/small_f90.dat
Conc
Time

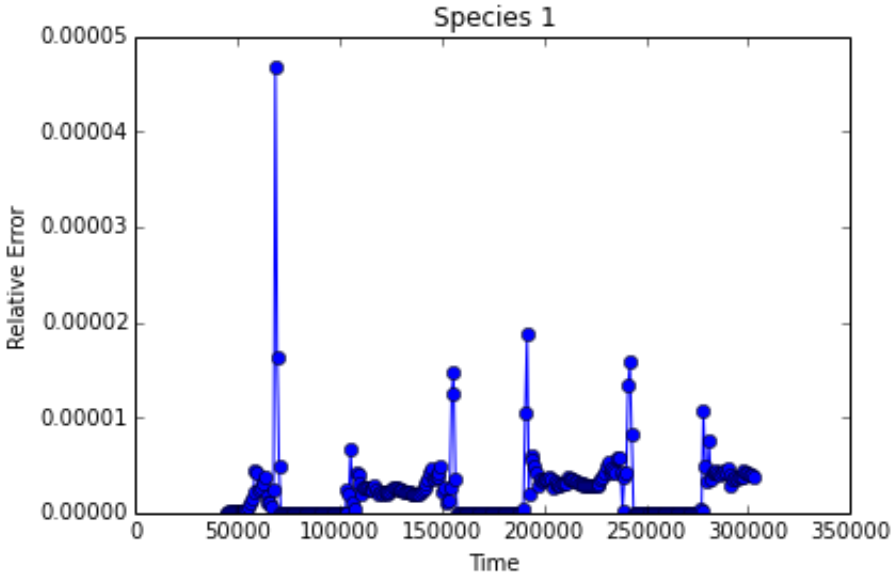


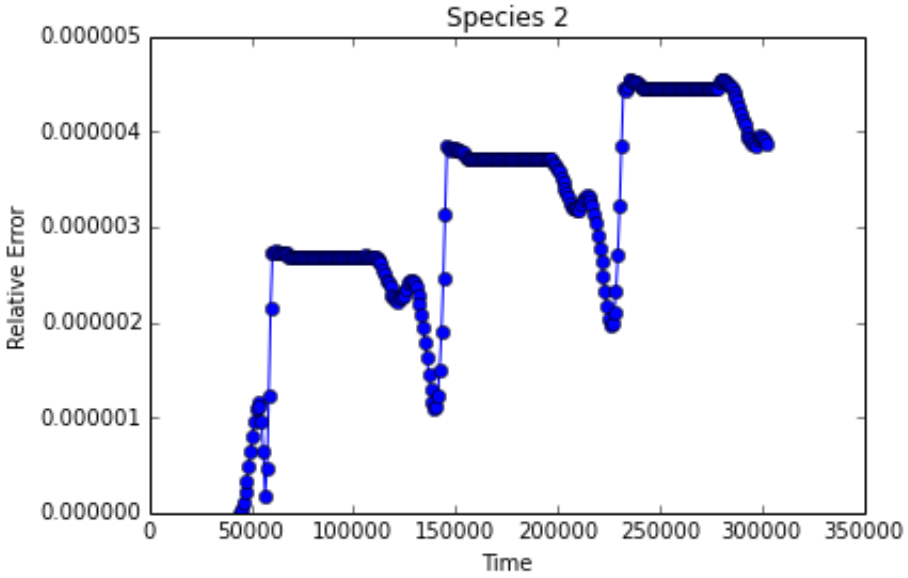
Results: Error vs. Time

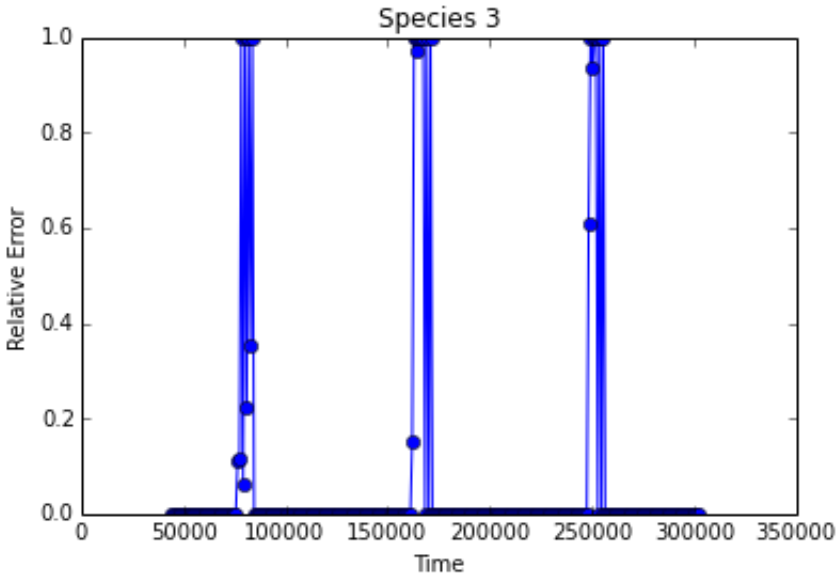
The following charts show relative error between the two data files vs. time.

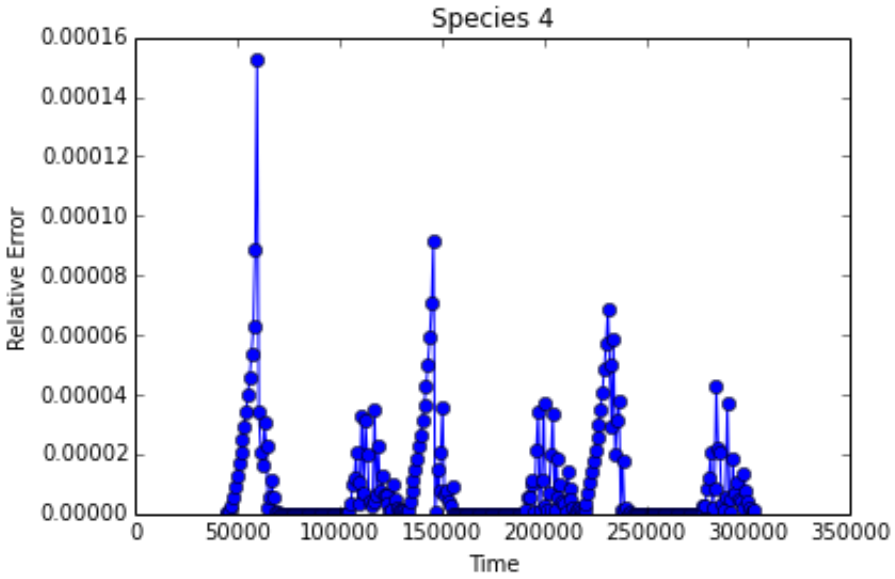
In [135]:
```
plot_dat([err_dat], ylabel='Relative Error')
```

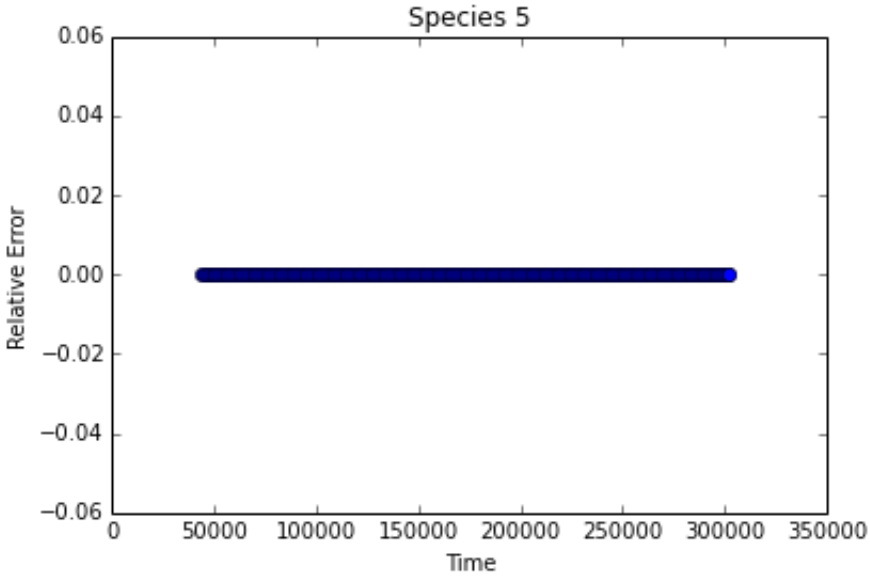


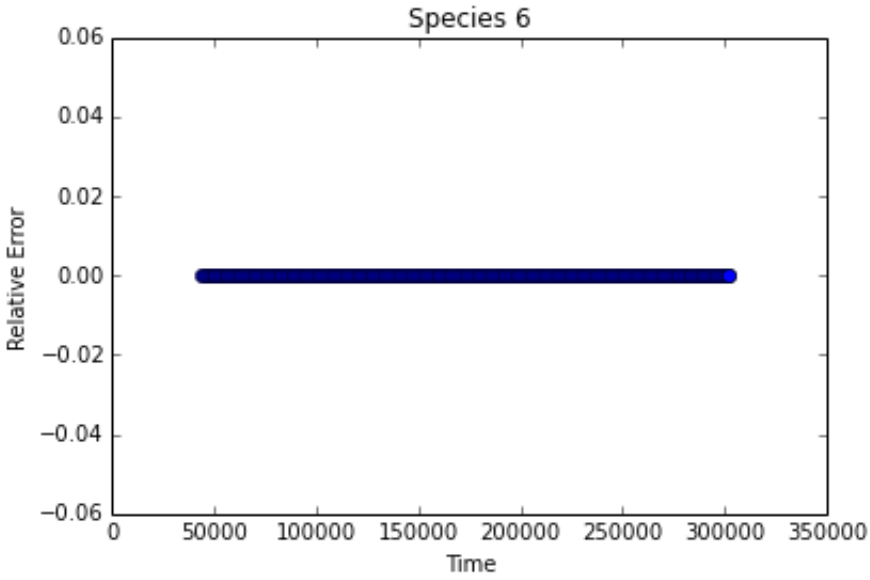

Species 1
Relative Error
Time
0.00005
0.00004
0.00003
0.00002
0.00001
0.00000
0
50000
100000
150000
200000
250000
300000
350000


Species 2
Relative Error
Time
0.000005
0.000004
0.000003
0.000002
0.000001
0.000000
0
50000
100000
150000
200000
250000
300000
350000


Species 3
Relative Error
Time
1.0
0.8
0.6
0.4
0.2
0.0
0
50000
100000
150000
200000
250000
300000
350000


Species 4
Relative Error
Time
0.00016
0.00014
0.00012
0.00010
0.00008
0.00006
0.00004
0.00002
0.00000
0
50000
100000
150000
200000
250000
300000
350000


Species 5
Relative Error
Time
0.06
0.04
0.02
0.00
−0.02
−0.04
−0.06
0
50000
100000
150000
200000
250000
300000
350000


Species 6
Relative Error
Time
0.06
0.04
0.02
0.00
−0.02
−0.04
−0.06
0
50000
100000
150000
200000
250000
300000
350000

In [107]: