Project 1, chemical reaction

$$\frac{dn_A}{dt} = -k_{AB}n_An_B + k_Cn_C$$

$$\frac{dn_B}{dt} = -k_{AB}n_An_B + k_Cn_C$$

$$\frac{dn_C}{dt} = k_{AB}n_An_B - k_Cn_C$$

```
na=na+dt*(-kab*nao*nbo+kc*nco )
nb=nb+dt*(-kab*nao*nbo+kc*nco )
nc=nc+dt*(+kab*nao*nbo-kc*nco )
```

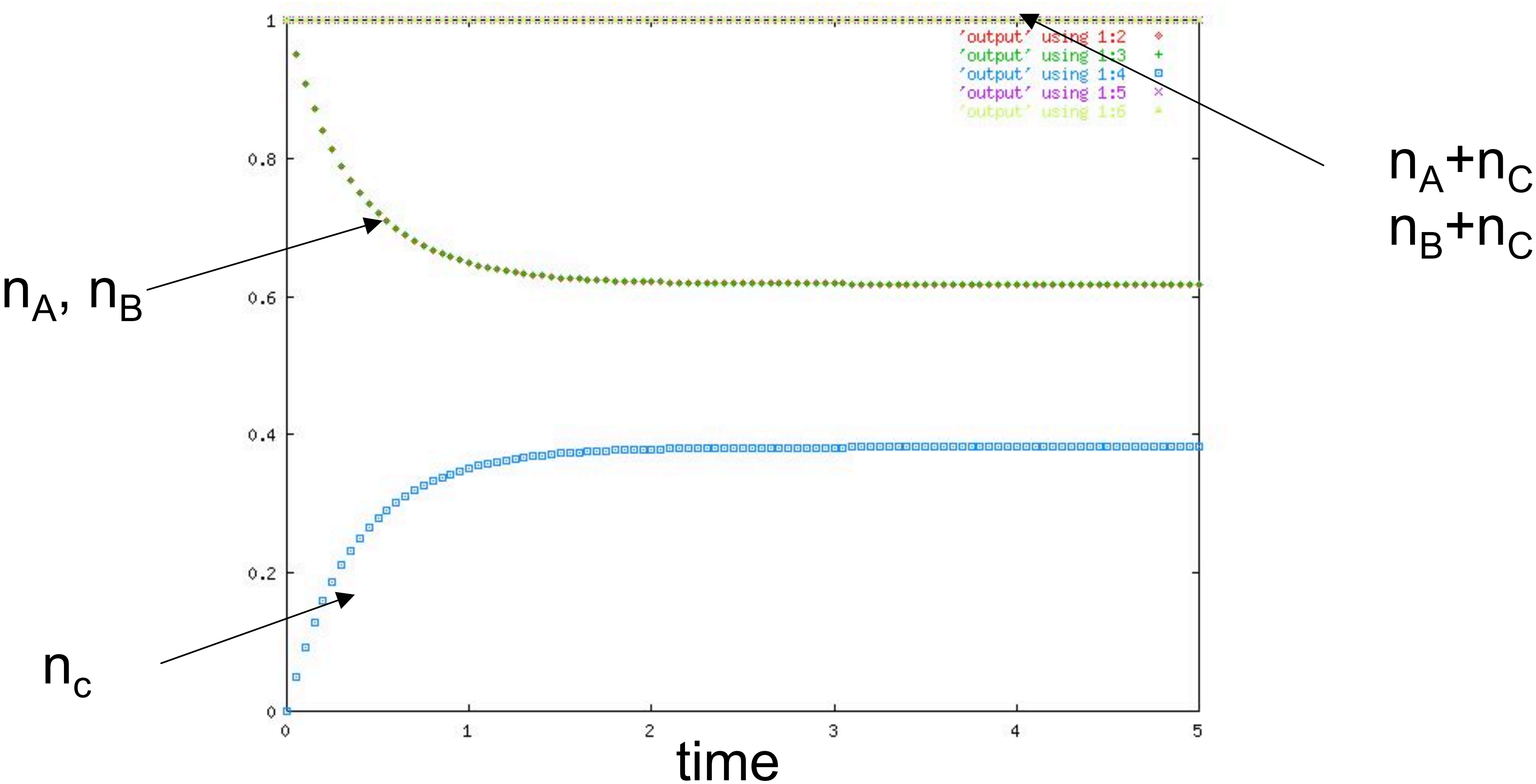
- $n_A + n_C$, $n_B + n_C$ constant
- Equilibrium at $n_An_B/ n_C = k_C/k_{AB}$

Project 1, plotting the results

Plotting results with gnuplot:

```
gnuplot> set term jpeg
Terminal type set to 'jpeg'
Options are 'small size 640,480 '
gnuplot> set output 'react.jpg'
gnuplot> plot 'output' using 1:2,'output' using 1:3, 'output' using 1:4,
'output' using 1:5,'output' using 1:6
gnuplot> quit
```

Project 1, Results for n_A=n_B=1, n_C=0 at t=0



- Run confirms $n_A+n_C = 1$, $n_B+n_C = 1$ for all times
- Final state agrees with $n_A n_B / n_C = k_C/k_{AB}$
- dt=0.05 adequate for $k_{AB}=k_C=1$ (reaction time ~ 1)

Next project…. Damped, driven oscillator

- Start with the case where q=0, F_D=0

$$\frac{d^2y}{dt^2} + \omega_0^2 y = 0$$

- y(t)= Acos ω_0t + Bsin ω_0t
- Initial conditions, A=y_0, B=v_0 / ω_0
- Energy (kinetic + potential should be conserved!

Compare with analytical to verify code, also test energy conservation!

Code prog3.f provide starting point… test!

$$\frac{d^2y}{dt^2} + \omega_0^2 y = 0$$

- Use Verlet algoritim

$$y_{n+1} = 2y_n - y_{n-1} - \omega_0^2 dt^2 y_n$$

```
c force/mass from spring
      force = -om0**2*ynow
c integrate to get y at next time step, use Verlet
      ynext = 2.0d0*ynow-ylast+dt**2*force
```

Initial conditions, analytic solution

- Analytic result computed for comparison
- Verlet algorithm needs position at two previous times
- Translate into initial position and initial velocity

$$y(t)= A\cos \omega_0 t + B\sin \omega_0 t$$

Initial conditions, $A=y_0$, $B=v_0 /\omega_0$

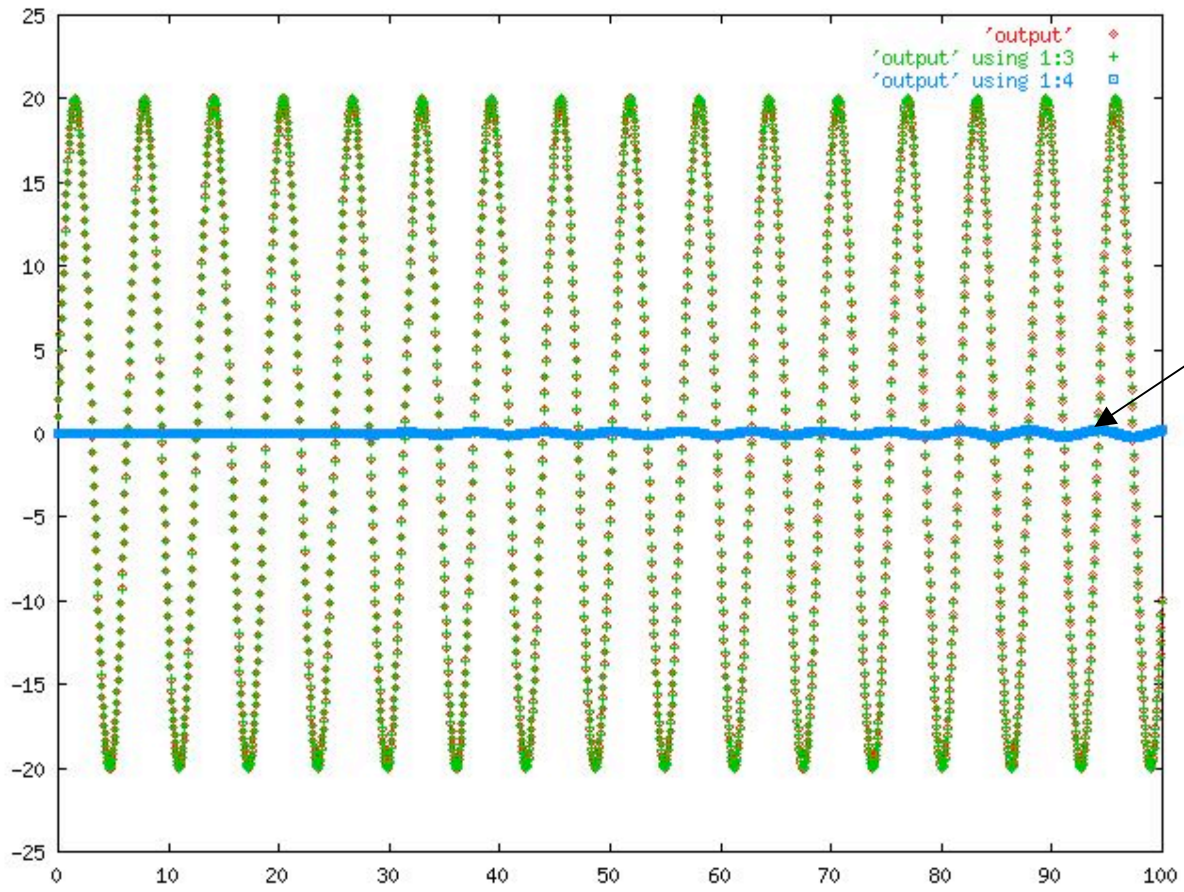
```
c velocity at current timestep
      vnow = (ynext-ylast)/(2.0d0*dt)
c If i=1 (first integration step), determine the initial conditions for an
c Next five lines not used in the case of damped, driven oscillator
      if(i.eq.1) then
        A=ynow
        B=vnow/om0
      endif
```

Energy calculation, analytical, and output

```
c velocity at current timestep
        vnow = (ynext-ylast)/(2.0d0*dt)


      potential = 0.5d0*sk * ynow**2
      kinetic = 0.5d0*vnow**2
      etot = potential + kinetic
      write (6,100) t,ynow,yanalytic,diff,potential,kinetic,
     :             etot
100    format(f8.4,6(2x,f12.6))
```

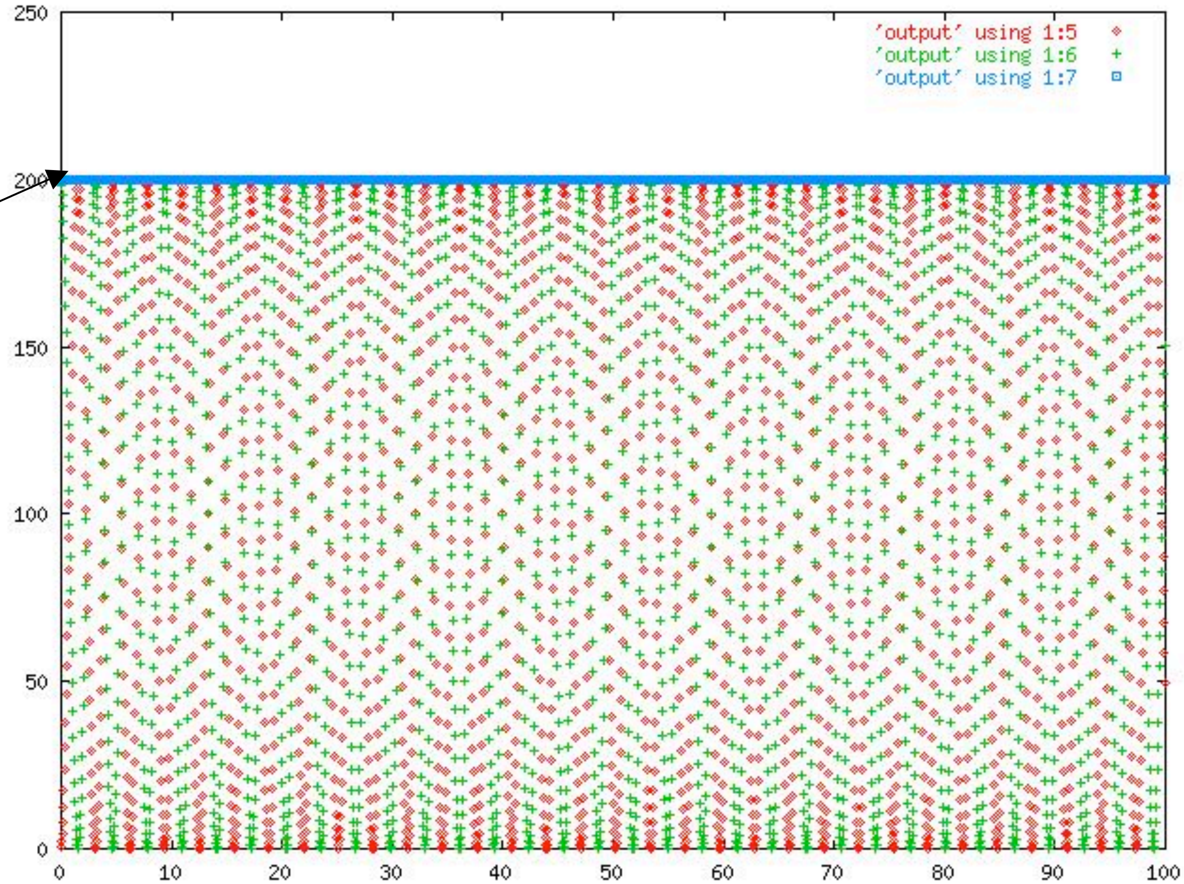
For $\omega_0 = 1, dt=0.05$



Difference between exact and numerical

gnuplot> set term jpeg
Terminal type set to 'jpeg'
Options are 'small size 640,480 '
gnuplot> set output 'displace.jpg'
gnuplot> plot 'output','output' using 1:3,'output' using 1:4

Energy conservation, potential, kinetic, total



Total energy conserved!

gnuplot> set output 'energy.jpg'
gnuplot> plot 'output' using 1:5,'output' using 1:6,'output' using 1:7

Damped, driven harmonic oscillator

$$\frac{d^2y}{dt^2} + 2q\frac{dy}{dt} + \omega_0^2 y = F_D cos\Omega_D t$$

- Have to work out numerical integration using Verlet!
- Case with q=0, F_D=0 serves as starting point
- Damping, driving force mean energy not conserved
- Can still compare to analytical y(t) after transient decays

In the underdamped regime, $q < \omega_0$

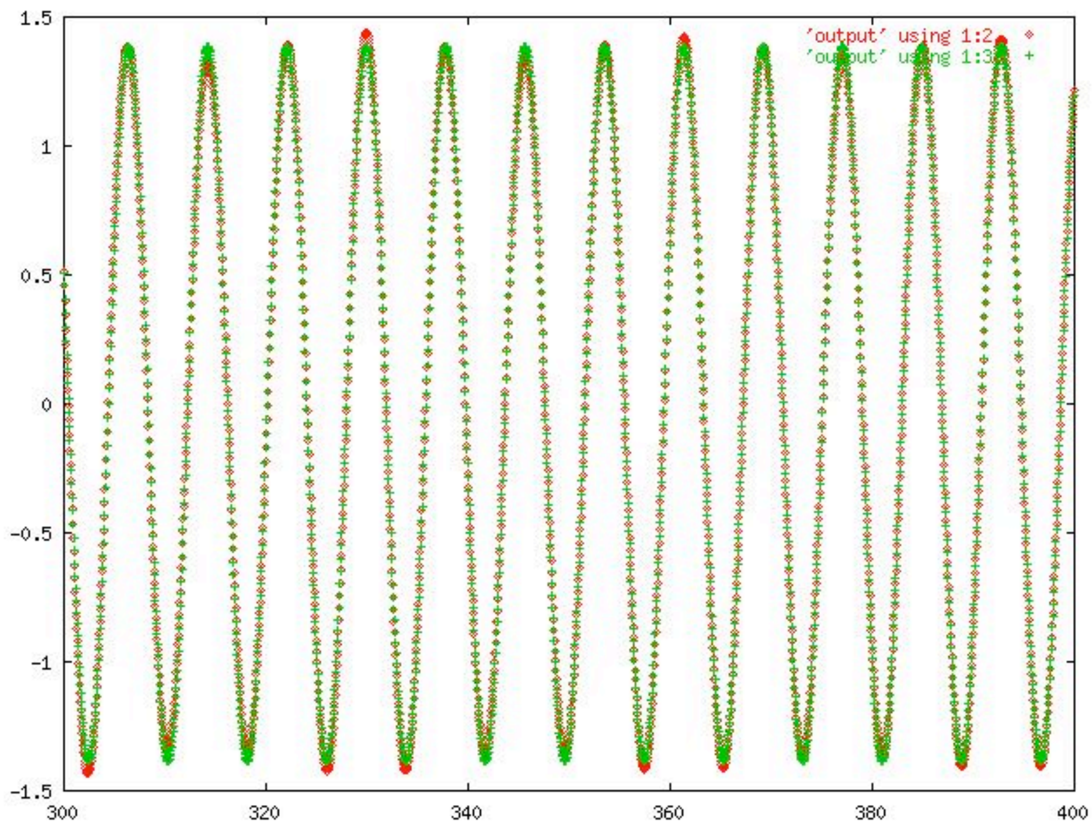
$$y(t) = c\ e^{-qt} \sin(\beta t + \phi)$$

For q=0.01, ω_0=1, transient decays away τ=1/q = 100

After decay of transient, analytical behavior is

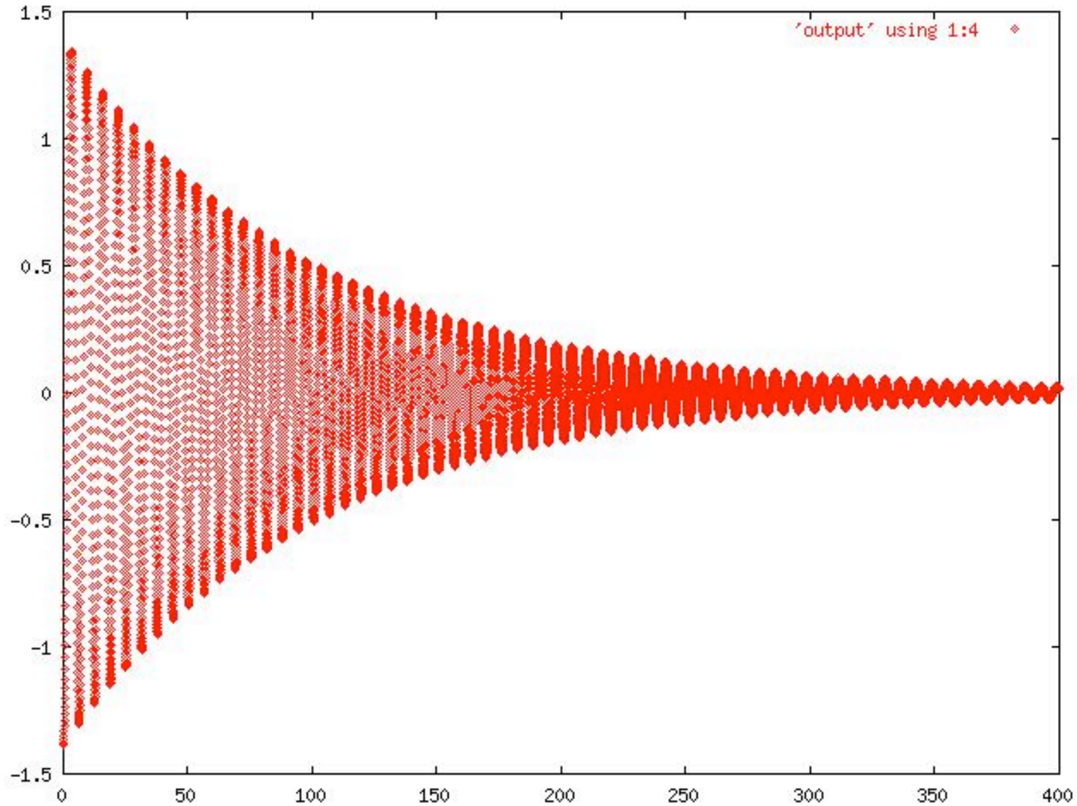
$$y(t) = A \sin(\Omega_D t - \gamma)$$

Damped, driven oscillator, position vs. time



Terminal type set to 'jpeg'
Options are 'small size 640,480 '
gnuplot> set output 'damped1.jpg'
gnuplot> plot [300:400] 'output' using 1:2,'output' using 1:3

Differences between analytic, numerical are due to transients, important for t<100



Differences are equal to the transient behavior, which is not included in analytical result in code

gnuplot> set output 'damped2.jpg'
gnuplot> plot 'output' using 1:4

Code for the analytical result, comparison

```
c Next three lines are for the damped, driven harmonic oscillator
c       A = F/dsqrt((om0**2-om**2)**2+(2.0d0*q*om0)**2) ! used for d
c       phi = datan(2.0d0*om*q/(om0**2-om**2)) ! used for damped d
c       yanalytic = A*dcos(om*t-phi) ! used for damped driven oscillat
       diff = ynow - yanalytic
```

Notice the transient behavior, which depends on the initial conditions, is not included here which explains the differences seen in the preceding slide

Uncomment these lines for project!

Nonlinear pendulum/oscillator

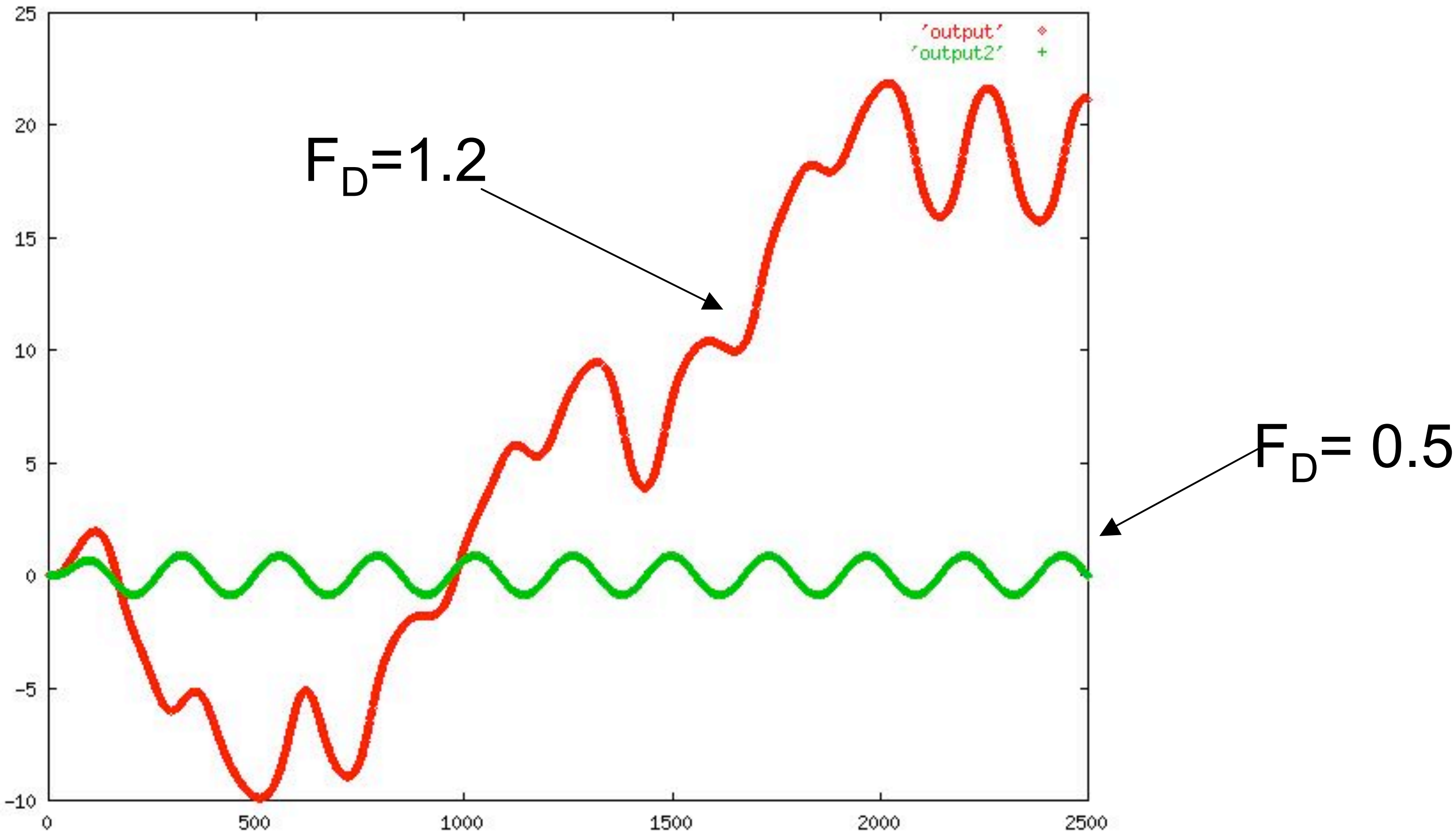
$$\frac{d^2y}{dt^2} + 2q\frac{dy}{dt} + \omega_0^2 \sin y = F_D cos\Omega_D t$$

- Large forces lead to chaotic behavior
- Predictable… but aperiodic…
- Slight differences in starting conditions lead to different response
- Analytical solution at least in closed form not possible!
- Superposition doesn't work as in linear case!

Nevertheless, small driving forces lead to linear, periodic response!

Simulation for two different driving forces…

$\Omega_D = (2/3)\omega_0$, q=1/2



- Initial position, velocity was zero
- Chaotic for larger driving force