Computational Modeling of Materials Homework III:

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Oscillatory Motion and Chaos

1.

$$\frac{d^2\theta}{dt^2} = -\frac{g}{l}\theta - 2\gamma\frac{d\theta}{dt} + \alpha_D \sin(\Omega_D t)$$

To analytically solve this, we will employ the small angle approximation as follows:

$$\frac{d^2\theta}{dt^2} = -\frac{g}{l}\theta - 2\gamma\frac{d\theta}{dt} + \alpha_D \Omega_D t$$

Now we can begin to solve this differential equation.

$$\frac{d^2\theta}{dt^2} + 2\gamma\frac{d\theta}{dt} + \frac{g}{l}\theta = \alpha_D \sin(\Omega_D t)$$

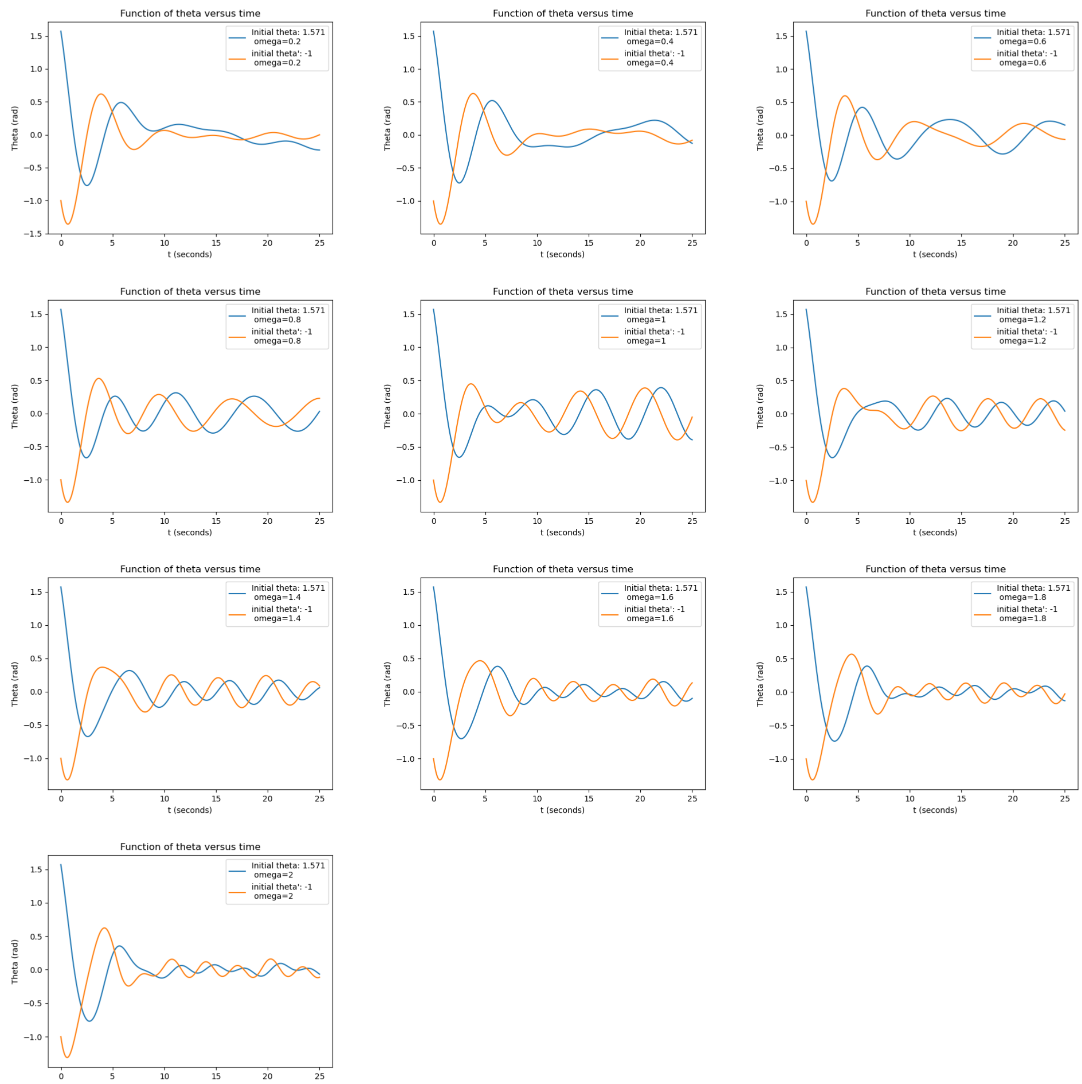
We'll begin with identifying that this is a second order non-homogeneous linear equation. We now know that in order to solve this problem, we must find the characteristic equation of the homogeneous characteristic equation.

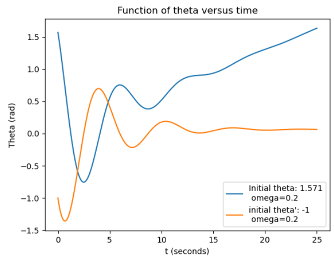
$$\theta_{homo} = c_1 e^{r_1 t} + c_2 e^{r_2 t}$$
$$r = \frac{-\gamma \pm \sqrt{\gamma^2 - 4\frac{g}{l}}}{2}$$

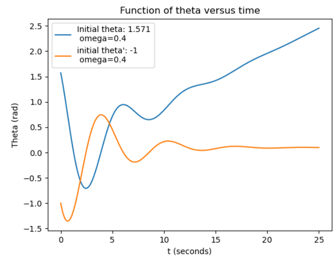
$$r = \frac{-0.25 \pm \sqrt{(0.25)^2 - 4\frac{9.8}{9.8}}}{2}$$
$$r = -\frac{1}{8} \pm \frac{\sqrt{-3.875}}{2}$$
$$r = -\frac{1}{8} \pm 0.984i$$
$$\theta_{homo} = e^{-\frac{t}{8}}(c_1 \sin(0.984t) + c_2 \cos(0.984t))$$

Now that we have the homogeneous solution, we can solve for the forcing function.

2-4




Function of theta versus time
Theta (rad)
t (seconds)
Initial theta: 1.571
omega=0.2
initial theta': -1
omega=0.2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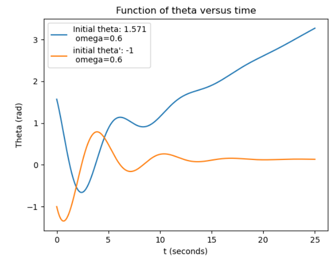
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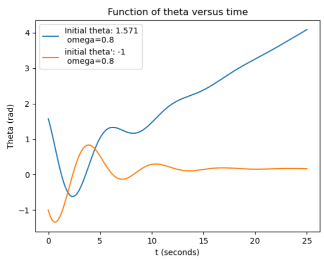
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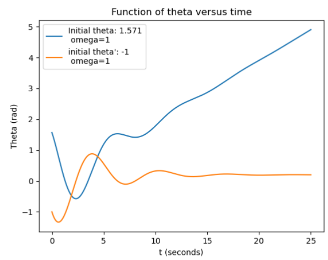
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t (seconds)
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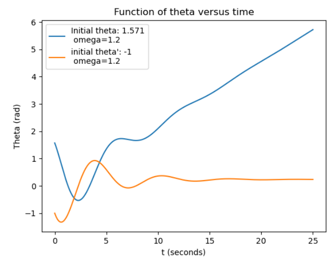
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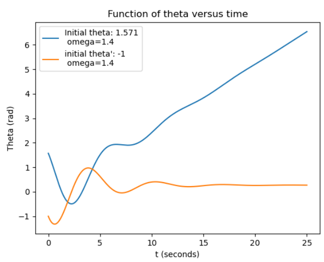
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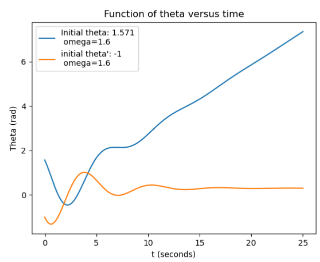
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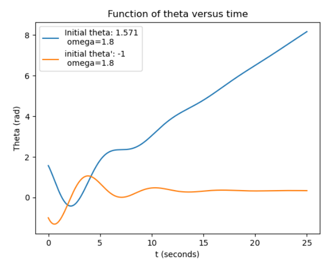
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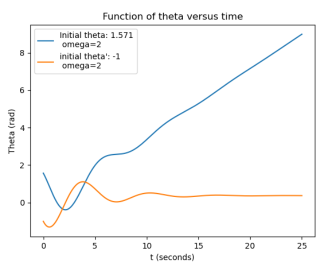
Function of theta versus time
Theta (rad)
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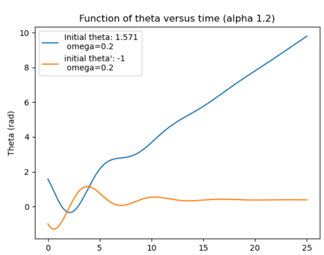
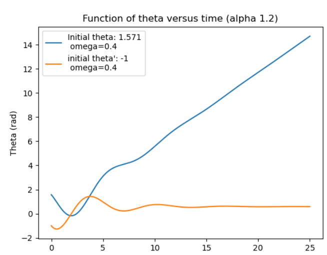
Initial theta: 1.571
omega=2
initial theta': -1
omega=2


Function of theta versus time (alpha 1.2)
Theta (rad)
t (seconds)
Initial theta: 1.571
omega=0.2
initial theta': -1
omega=0.2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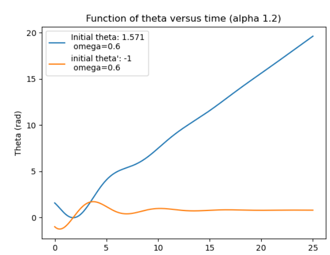
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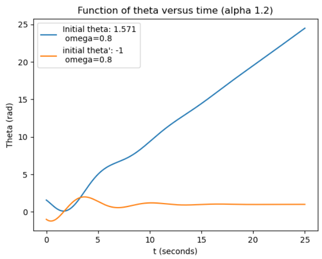
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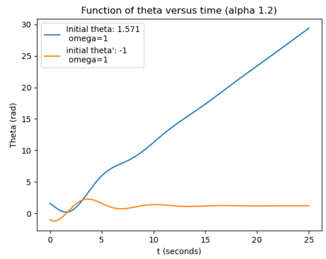
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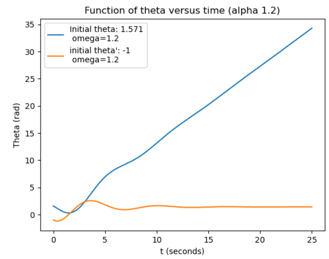
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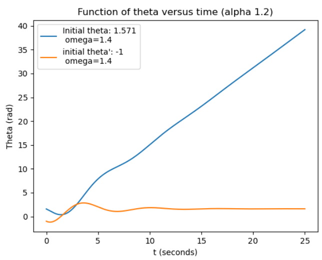
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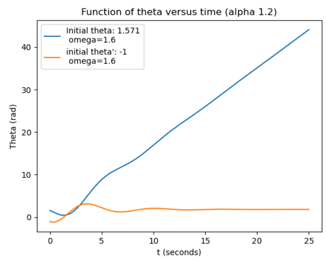
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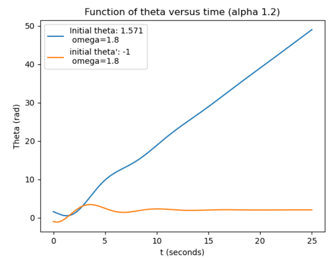
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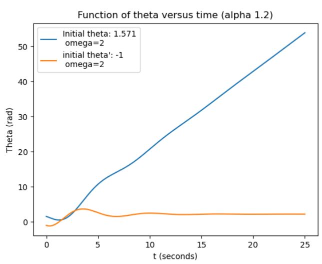
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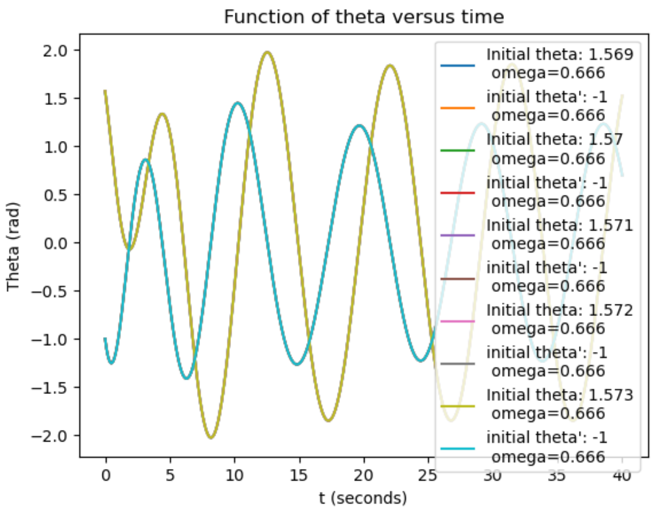
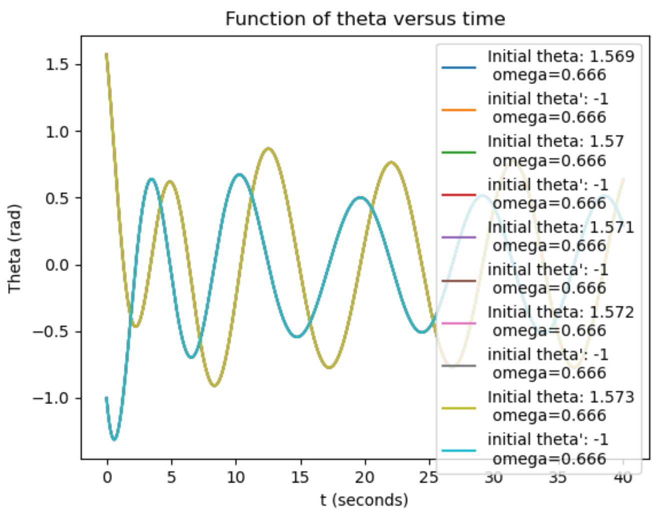
initial theta': -1
omega=2
Theta (rad)
t (seconds)

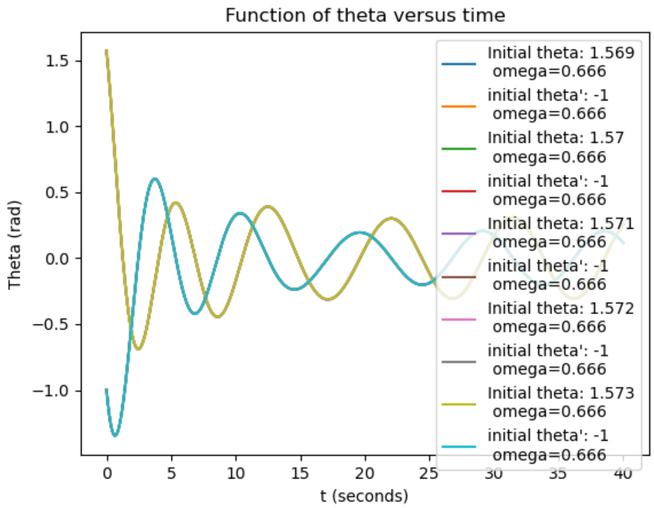
5.



Graph where $\alpha = 1.2$



Graph where $\alpha = 0.5$

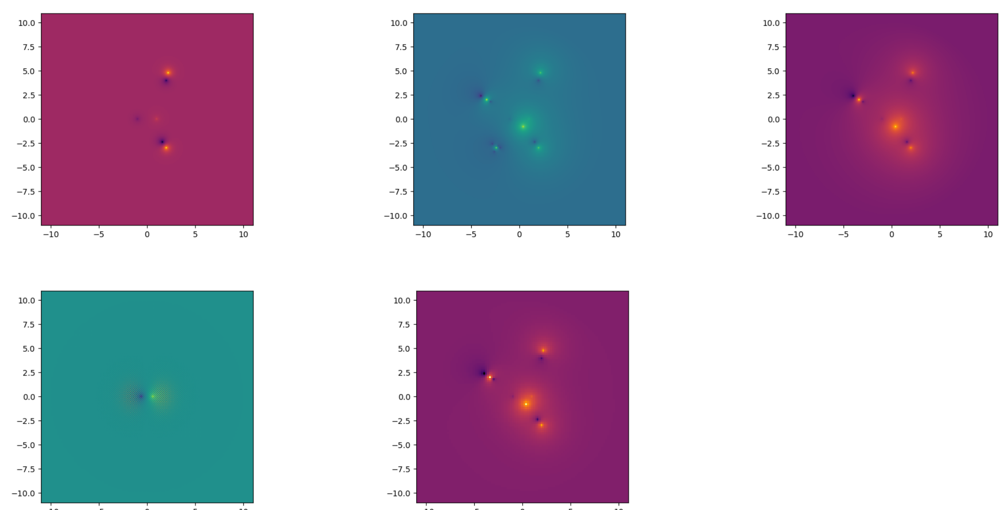


Graph where $\alpha = 0.2$

Discussion

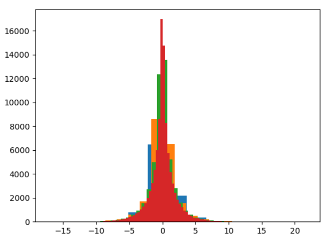
Now we can see how the impact of slight changes, as well as values closer to the resonant frequency, impact overall oscillation. We can see that a few tweaks to values can cause major long term behavioral changes.

Poisson Equation for Dipole



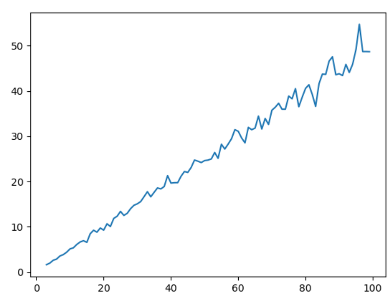
Here multiple point charges are used, but the same image is conveyed. It can be apparent to the reader which models have run for longer, and which have converged. The SOR model, oddly, converged more slowly. For a standard grid with dx=0.2 it took around 3777 iterations to converge for Jacobi, whereas, SOR took much longer to.

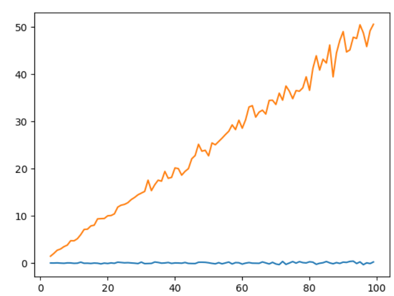
Random Numbers



We can now see in this part that the algorithm we generated did indeed work as we have received the gaussian distribution.

2D Random Walk





Here we can see the magnitude of the walk as well as the overall displacement. As expected, we can see that $\langle r^2 \rangle$ is indeed proportional to t by a factor of approximately 2.

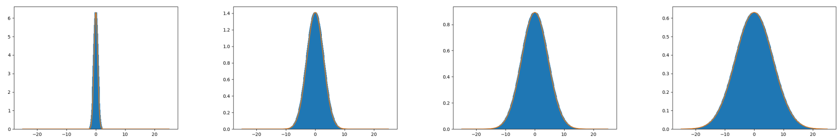
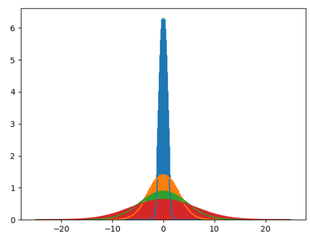
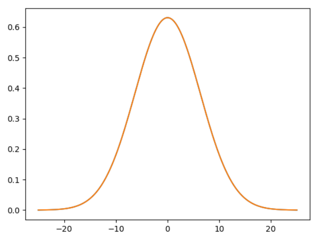


Figure 1: Diffusion at t=2,5,10,20

1D Diffusion





1.

$$\rho(x,t) = \frac{1}{\sqrt{2\pi\sigma(t)^2}} e^{\left(-\frac{x^2}{2\sigma(t)^2)}\right)}$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 \rho(x,t) dx$$

$$\langle x^2 \rangle = \frac{1}{\sqrt{2\pi\sigma(t)^2}} \int_{-\infty}^{\infty} e^{\left(-\frac{x^2}{2\sigma(t)^2)}\right)} x^2 dx$$

Since we know:

$$\int_{-\infty}^{\infty} x^2 e^{-x^2} dx = \frac{\sqrt{\pi}}{2}$$

...and:

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{2a^{3/2}}$$

We can plug in values as follows:

$$a = \frac{1}{2\sigma(t)^2}$$

$$\langle x^2 \rangle = \frac{1}{\sqrt{2\pi\sigma(t)^2}} \int_{-\infty}^{\infty} e^{\left(-\frac{x^2}{2\sigma(t)^2)}\right)} x^2 dx$$

$$\langle x^2 \rangle = \frac{1}{\sqrt{2\pi\sigma(t)^2}} \cdot \left(\frac{\sqrt{\pi}}{2(2\sigma(t)^2)^{3/2}}\right)^{-1} dx$$

$$\langle x^2 \rangle = \frac{1}{\sqrt{2\pi\sigma(t)^2}} \cdot \frac{\sqrt{\pi}(2\sigma(t)^2)^{3/2}}{2}$$

$$\langle x^2 \rangle = \frac{1}{\sqrt{2\pi\sigma(t)^2}} \cdot \frac{\sqrt{8\pi}\sigma(t)^3}{2}$$

$$\langle x^2 \rangle = \frac{1}{\sqrt{2\pi}\sigma(t)} \cdot \frac{2\sqrt{2\pi}\sigma(t)^3}{2}$$

$$\langle x^2 \rangle = \sigma(t)^2$$

2.

As can be seen above, diffusion over time can be seen to indeed fit the normal distribution.

Extra Credit Gases

Code inside submission.

Acknowledgments

Work within the group was done with collaboration for concepts, while coding was all done individually.