Scaling differential equations to dimensionless variables:

There are several reasons to scale differential equations before implementing them numerically.

- Computers know nothing of units, they only work with numbers. It makes sense then to scale equations to dimensionless numbers.
- Physical quantities can vary over many orders of magnitude. Since computers work to finite accuracy, it makes sense to scale units so that calculations involve numbers of reasonable magnitudes.
- Clever scaling can reduce the number of parameters in your problem so that your solutions are more general. If your problem has two parameters, A and B, you might want to study solutions for 10 different values of A and 10 different values of B for each value of A, or 100 runs. But if the scaled problem only depends upon the ratio A/B, you might only do 10 runs.
- Clever scaling can reveal underlying physics of your problem, indicating what it means to have a "strong" coupling in a system, or what it means for two particles to be "far apart."

There are five steps in turning a problem into dimensionless variables. They are:

1. Replace each *independent variable* by a product of a dimensionless variable and a constant that carries the units.
2. For each scaling constant see if there is a choice that you can make that will set the coefficient of two terms equal to the same quantity. However, don't:
    a. Include factors of $i = \sqrt{-1}$ or "-1" when making your choice of scaling, since that can change the nature of the solutions you find (e.g. oscillating to exponentially growing).
    b. Choose a value of the scaling constant that will diverge in some limit you want to explore.
3. Divide out this common coefficient from all terms. If you have done this correctly, *all* coefficients are now either pure numbers or dimensionless ratios.
4. If you have any remaining scaling constants, see if you can chose their value so that one of the dimensionless ratios becomes unity (the number "1").
5. Examine the remaining terms to see if:
    a. Scaling the *dependent* variables will give a simpler expression.
    b. Scaling any eigenvalues will give a simpler expression.

Don't blindly introduce scaling to every quantity in your equation. You are trying to simplify the results, not make them more complicated.

Let's do an example.

Scaling the quantum harmonic oscillator equation

Consider the partial differential equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + \frac{1}{2}kx^2\,\psi(x) = E\,\psi(x)$$

Step 1: We have one independent variable, x. We introduce the scaling $x = x_o\, s$, where s is the dimensionless distance and x_0 carries the units.

$$-\frac{\hbar^2}{2mx_0^2}\frac{\partial^2}{\partial s^2}\psi(s) + \frac{1}{2}kx_0^2\, s^2\,\psi(s) = E\,\psi(s)$$

Note that we don't scale ψ since every term has a ψ in it and we don't gain anything. We also don't scale *m, k,* or any other constant in the problem. Now the trick is to find a good choice for x_0 so that we can simplify the equation. We want to set two terms to the same value so that we can cancel the common factor. Possible choices:

- $\frac{\hbar^2}{2mx_0^2} = \mathrm{E}$ This won't help since we don't know the value of *E*, the energy. It's one of the things we are trying to find, so we don't want it to disappear from the equation.
- $\frac{1}{2}\mathrm{kx}_0^2 = \mathrm{E}$ Again, not a help.
- $\frac{\hbar^2}{2mx_0^2} = \frac{1}{2}\mathrm{kx}_0^2$ This works!

Solving this equation for the value of x_0 we find that $\mathrm{x}_0^2 = \hbar/\sqrt{\mathrm{km}}$. Substituting it back into our equation we get:

$$-\frac{1}{2}\hbar\sqrt{\frac{k}{m}}\frac{\partial^2}{\partial s^2}\psi(s) + \frac{1}{2}\hbar\sqrt{\frac{k}{m}}\, s^2\,\psi(s) = E\,\psi(s)$$

Now we can see a common factor of $\frac{1}{2}\hbar\sqrt{\mathrm{k/m}}$, which you might recognize as $\frac{1}{2}\hbar\omega_0$. At this point we can divide through by this quantity and get:

$$-\frac{\partial^2}{\partial s^2}\psi(s) + s^2\,\psi(s) = \frac{E}{\frac{1}{2}\hbar\omega_0}\,\psi(s)$$

(Note that we could have left the factor of ½ on the left hand side of the equation if we wanted to do so – some texts leave it in the differential equation). Finally we see that we can further simplify this equation if we choose to measure energy in units of $\frac{1}{2}\hbar\omega_0$:

$$E = (\frac{1}{2}\hbar\omega_0)\,\epsilon$$

where ϵ is the dimensionless energy variable and so our equation is much simpler. Our final equation is:

$$-\frac{\partial^2}{\partial s^2}\psi(s) + s^2\,\psi(s) = \epsilon\,\psi(s)$$

which is much simpler than our original differential equation.

While this choice of scaling is absolute acceptable and is, in fact, the one found in most quantum mechanics textbooks, it might not be the best choice for some numerical problems. By chosing x_0 in this fashion, our ruler depends upon the strength of the spring constant *k* and the particle mass *m*. It might be that for *physical* reasons (as opposed to mathematical ones), we want to confine the system in a box of width *L* so that $\psi(-L/2) = \psi(L/2) = 0$, where *L* is some physical, dimensioned length. In that case the above choice of x_0 would mean that our box would change size (in the dimensionless variable *s*) when we change the spring constant or mass of the particle. In this second case it makes more sense to set $x_0 = L$. Our equation becomes:

$$-\frac{\hbar^2}{2mL^2}\frac{\partial^2}{\partial s^2}\psi(s) + \frac{1}{2}kL^2\,s^2\,\psi(s) = E\,\psi(s)$$

Now to simplify we can either divide the equation by $\hbar^2/2mL^2$ or by $kL^2/2$. However, we should check if this might cause problems. Let's further assume that we are interested in how the eigenenergies of the system change when we adjust *k*. In the limit *k=0,* we know that there is no longer a potential and we should recover the energies of the 1D particle-in-a-box states, since the boundary condition is effectively an infinite confining potential. This gives us a useful check on our answer (since we know the analytic result) and it might reflect a realistic physical limit if the restoring force could actually be turned off. This means we should *not* scale by $kL^2/2$, since that "ruler" vanishes when *k=0.*

Our equation now becomes:

$$-\frac{\partial^2}{\partial s^2}\psi(s) + \frac{\frac{1}{2}kL^2}{\frac{\hbar^2}{2mL^2}}\,s^2\,\psi(s) = \frac{E}{\frac{\hbar^2}{2mL^2}}\,\psi(s)$$

which looks like a bit of a mess, but is easy to clean up, if we measure energy in units of $\hbar^2/2mL^2$, and define the dimensionless force constant:

$$\delta = \frac{\frac{1}{2}kL^2}{\frac{\hbar^2}{2mL^2}}$$

Then our equation takes on the simple form:

$$-\frac{\partial^2}{\partial s^2}\psi(s) + \delta\, s^2\, \psi(s) = \epsilon\, \psi(s)$$

This looks similar to the form obtained above, but is not the same – our distance *s* is now defined in terms of the fixed length *L*, and the spring constant can now be "strong" or "weak". This is another important feature of scaling differential equations: **scaling can give insight into the physical features of the problem.** In this case we see that a "strong" spring constant is one for which the maximum potential energy of the particle is comparable to $\hbar^2/2mL^2$, which is the energy of a quantum particle in a box of width *L*, (up to a factor of π^2).

<u>Practice Example:</u>

Let's assume that you are interested in the time evolution of an initial wave packet that starts as a gaussian at the origin and obeys the time dependent Schrodinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V_0\, x\, \sin\omega t\, \psi(x,t) = -i\hbar\frac{\partial}{\partial t}\psi(x,t)$$

This is a potential that alternately slopes to the left and then to the right, possibly causing the particle to oscillate in position. How would you prepare to solve the problem by scaling the differential equation? What does it mean for the oscillation to be "fast" or "slow"?