Methods I:

Discretization of Ordinary Differential Eqns.

As a starting point consider a vector equation central to much of mechanics:

$$m\,\mathbf{a} = \mathbf{F}$$

In one dimension, say z, we know that we can often write this as an ordinary differential equation (ODE):

$$m\ d^2z / dt^2 = F(z, v, t)$$

For example, a mass on a spring in a viscous medium might have $F = kz - bv$. Further, by using the definition of velocity, the above *second* order ODE can be split into two, coupled *first* order ODEs:

$$dv / dt = F(z, v, t) / m \qquad \text{Eq. 1a}$$

$$dz / dt = v \qquad \text{Eq. 1b}$$

Each of these equations has the general form that we need now to consider:

$$dy / dx = f(y, x)$$

Given an initial condition such as $y(x_o=0) = y_o$, how can one solve such an equation -- determine y_{final} at some x_{final} -- if the function f is a complicated expression? The basic procedure is to *discretize over some small but finite time interval*, Δx, and "numerically integrate" with a first step:

$$(y_1 - y_o)/\Delta x \approx f(y_o, 0) \qquad \Rightarrow \qquad y_1 \approx y_o + f(y_o, 0) * \Delta x$$

This gives $y_1(x = x_1)$ in terms of known or set (Δx) quantities. The next step gives y_2 from:

$$y_2 \approx y_1 + f(y_1, x_1) * \Delta x$$

If you program a computer to do this, you would simply want to specify the number of steps, N, that you take from x=0 to $x=x_{final}$ and then employ the following relation in an iterated loop:

$$y_{n+1} \approx y_n + f(y_n, x_n) * \Delta x \qquad (n = 0, N)$$

The best numerical estimate of $y(x_{final})$ is typically obtained for largish N, but not too large.

Going back to the two, coupled first order ODEs above, the relations to be iterated are

$$v_{n+1} \approx v_n + (1/m)\, F(z_n, v_n, t_n) * \Delta t \qquad \text{Eq. 2a}$$

$$z_{n+1} \approx z_n + v_n * \Delta t \qquad \text{Eq. 2b}$$

To solve this for $v(t_{final})$ and $z(t_{final})$, one requires two initial conditions such as z(t=0) and v(t=0).

The above scheme for numerical integration is the very simplest and is known as Euler's method. Much can be found in the literature on better approximations for the iterative step. In addition, one does have to beware of numerical round-off errors (N large) and other noise or instability issues. A simple and a more thorough reference for such issues are, respectively:

Computational Physics by Steven E. Koonin, Ch. 2, Addison-Wesley Publishing, 1990.
Numerical Recipes by W.H. Press et al, Chs. 15-16, Cambridge Univ. Press, 1990.

NumPS#1-1. Extend your arm straight out and imagine having someone place into your hand an $m = 2.5$ kg mass (~5 lb). Your arm would naturally displace downward, and, if you tried to stop this motion, you would tend to exert an upward restoring force related to both your hand's velocity and its displacement. **(A)** Sketch a free body diagram for the mass and assume the 'active' response of your hand could be modeled as power laws in both displacement (kz^{κ}) and velocity (bv^{β}). **(B)** Write down for the mass the n=0 and n=1 finite difference equations (Eq. 2a,b) using suitable initial conditions and always neglecting the mass of your hand and arm. **(C)** Do you think that the various constants ($b,k,\ldots$) might depend on the strength and age of the person? Does this suggest any useful quantitative approaches to tests of a person's motive reflexes?

Barometric Formulas describe how the pressure or density of a fluid (particularly air) decreases with increasing height above a reference point (such as the ground).

The constitutive equation for air might be considered to be that of an ideal gas where

$$p = \rho\ (1/M_m)\ RT \qquad \text{Eq. 1a}$$

with ρ as the mass density and M_m the molar mass (air: 30 g/mol). Air might also be modeled as a van der Waals fluid:

$$p = \rho\ (1/M_m)\ RT\ /\ (1 - B\ \rho) - A\ \rho^2. \qquad \text{Eq. 1b}$$

In this latter equation, the constant A attempts to reflect a tendency for molecules to attract and condense (forming liquid) and the constant B reflects a tendency for molecules not to overlap in space. For nitrogen and argon, two major components of air, these constants are very well known.

The equations of static equilibrium for a cube of air at a position (x,y,z) above some reference point on the earth involve only the normal stresses. Since air is a fluid, it's static stresses depend only on density, and it therefore does not *statically* sustain shear stresses. Further assuming that gravity as well as temperature are independent of z, we get partial differential equations (PDE's) that reduce to

$$\partial\sigma_{xx}\ /\ \partial x = 0, \qquad \partial\sigma_{yy}\ /\ \partial y = 0, \qquad \partial\sigma_{zz}\ /\ \partial z - \rho\ g = 0 \qquad \text{Eq. 2}$$

Since $\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = -p$, the first two equations imply that the pressure is independent of x and y, as we should anticipate, so that p = p(z). The third equation above then implies that

$$dp\ /\ dz = -\ \rho\ g \qquad \text{Eq. 3}$$

If one assumes that air is an ideal gas, then the differential equation becomes

$$d\rho\ /\ dz = -\ \rho\ g\ /\ [\ (1/M_m)\ RT\ ] \qquad \text{Eq. 4a}$$

which integrates to

$$\rho(z) = \rho_o \exp[\ -\ z\ (M_m\ g\ /\ RT)\ ]$$

where $\rho = \rho_o$ (p_o = 1 atm if not compressed) at ground level, z = 0. However, if air is taken to be a van der Waals fluid, one has a more complicated differential equation to integrate

$$dp\ /\ dz = (\ dp\ /\ d\rho\ )\ (\ d\rho\ /\ dz\ )$$

$$= \{ (RT/M_m)/ (1 - B\rho) - \rho B (RT/M_m) / (1 - B\rho)^2 - 2 A \rho \} (d\rho / dz)$$

This implies an equation of the canonical form $dy / dx = f(y,x)$ where $x \to z$ and $y \to \rho$:

$$d\rho / dz = - \rho g / \{ (RT/M_m) / (1 - B\rho) - \rho B (RT/M_m) / (1 - B\rho)^2 - 2 A \rho \} \qquad \text{Eq. 4b}$$

Although this is analytically integrable, it is a good candidate for numerical integration especially if one also includes the feature that the van der Waal's fluid exhibits liquid-gas phase transitions.

NumPS#1-2. Integrate Eq. 4b analytically to determine a non-exponential form for $\rho(z)$ of a dense fluid.

Methods II:

Partial Differential Equations & Finite Differences

The first order ODE that yields the exponential barometric formula resulted from significant collapse of the governing PDE's primarily because stress is only a function of density and the body force has just one known component. However, very often in mechanics, PDE's of second or higher order must be solved numerically. Recall, for example, *Navier's equation* (Fung, pg. 272) in the static equilibrium limit (i.e. $\ddot{u}_i = 0$):

$$G\,[\,\nabla^2 u_i + (1-2\nu)^{-1}\,(\,\partial u_1/\partial x_1 + \partial u_2/\partial x_2 + \partial u_3/\partial x_3\,)_{,i}\,] + \rho b_i = 0$$

This was obtained from the equations of motion, i.e. $\sigma_{ji,j} + \rho b_i = \rho \ddot{u}_i$, involving a first derivative of stress, i.e. $\sigma_{ij}(x,y,z)$, and, through constitutive relations between σ_{ij} and $\varepsilon_{ij} = (u_{i,j} + u_{j,i}) / 2$, whereby derivatives of the displacement field entered the picture. To approach such PDE's numerically, we present here only the most introductory ideas that extend the previous ODE ideas to, first, higher order derivatives, i.e. u'', and then functions of more than one variable, eg. u(x,y).

Our starting point is the approximation previously introduced for ODE's:

$$y_{n+1} \approx y_n + f(x_n, y_n) * \Delta x$$

Noting that $f = y'$, we rewrite the above and generalize it slightly to calculate y-values at points on either side of the nth point

$$y_{n\pm1} \approx y_n \pm \Delta x * y'(x_n, y_n)$$

Importantly, this has the form of a Taylor series (i.e. $y(x) = y(x_o) + \Delta x\, y' + (\Delta x^2 / 2!)\, y'' + ...$),

which suggests higher order approximations

$$y_{n+1} \approx y_n + \Delta x * y'(x_n, y_n) + (\Delta x^2 / 2!) * y''(x_n, y_n)$$

$$y_{n-1} \approx y_n - \Delta x * y'(x_n, y_n) + (\Delta x^2 / 2!) * y''(x_n, y_n)$$

Adding these together gives

$$y_{n+1} + y_{n-1} \approx 2y_n + \Delta x^2 * y''(x_n, y_n)$$

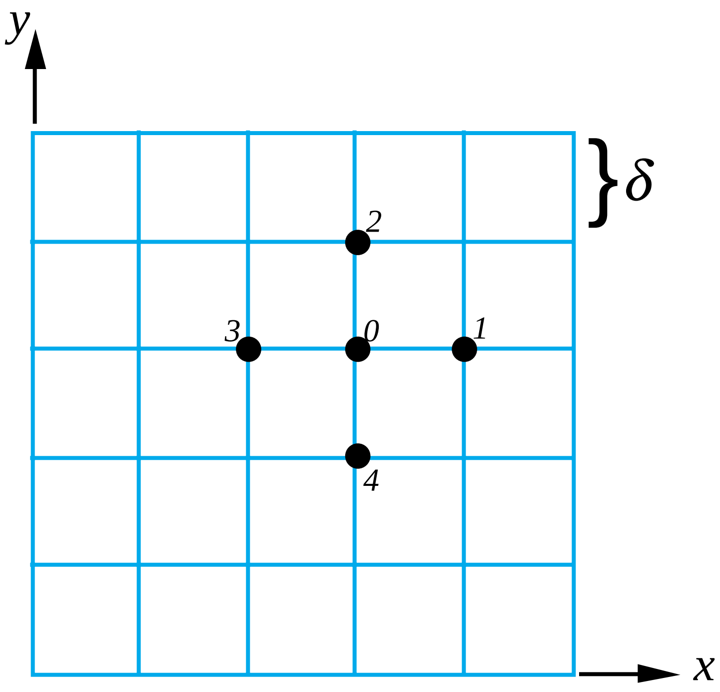
Rearranging this we obtain an approximation for the second derivative of a function at the nth point in terms of function values at neighboring points:

$$y''(x_n, y_n) \approx (y_{n+1} - 2y_n + y_{n-1}) / \Delta x^2$$

PDE's, by definition, involve functions of more than one variable, functions such as u(x,y). Recall from calculus the Taylor series expansions for such functions

$$\begin{aligned} u(x,y) = u(x_o, y_o) + \Delta x\,(\partial u/\partial x) + (\Delta x^2 / 2!)\,(\partial^2 u/\partial x^2) \,+& \\ \Delta y\,(\partial u/\partial y) + (\Delta y^2 / 2!)\,(\partial^2 u/\partial y^2) + (\Delta x\,\Delta y)\,(\partial^2 u/\partial x\partial y) + \ldots& \end{aligned}$$

On the square gridded domain below, for convenience, $\Delta x = \Delta y = \delta$, and we've also labeled the n^{th} node with a zero.



The finite difference approximations for the unmixed partial derivatives at the point (x_o, y_o) on such a grid are deduced by addition, subtraction, and reaarangment of the following four equations:

$$u_1 \approx \mathbf{u_o} + \boldsymbol{\delta\,(\partial u/\partial x) + (\delta^2 / 2!)\,(\partial^2 u/\partial x^2)} + 0\,(\partial u/\partial y) + (0^2 / 2!)\,(\partial^2 u/\partial y^2) + (\delta * 0)\,(\partial^2 u/\partial x\partial y)$$

$$u_3 \approx \mathbf{u_o} \boldsymbol{- \delta\,(\partial u/\partial x) + (\delta^2 / 2!)\,(\partial^2 u/\partial x^2)} + 0\,(\partial u/\partial y) + (0^2 / 2!)\,(\partial^2 u/\partial y^2) + (\delta * 0)\,(\partial^2 u/\partial x\partial y)$$

$$u_2 \approx \mathbf{u_o} + 0\,(\partial u/\partial x) + (0^2 / 2!)\,(\partial^2 u/\partial x^2) + \boldsymbol{\delta\,(\partial u/\partial y) + (\delta^2 / 2!)\,(\partial^2 u/\partial y^2)} + (\delta * 0)\,(\partial^2 u/\partial x\partial y)$$

$$u_4 \approx \mathbf{u_o} - 0\,(\partial u/\partial x) + (0^2 / 2!)\,(\partial^2 u/\partial x^2) \boldsymbol{- \delta\,(\partial u/\partial y) + (\delta^2 / 2!)\,(\partial^2 u/\partial y^2)} + (\delta * 0)\,(\partial^2 u/\partial x\partial y)$$

The non-zero terms in bold then yield:

$$\partial u_o / \partial x \approx (u_1 - u_o) / \delta$$

$$\partial u_o / \partial y \approx (u_2 - u_o) / \delta$$

$$\partial^2 u_o / \partial x^2 \approx (u_1 - 2u_o + u_3) / \delta^2$$

$$\partial^2 u_o / \partial y^2 \approx (u_2 - 2u_o + u_4) / \delta^2$$

As is necessary to rewrite Navier's equation in finite difference form, the mixed partial derivatives must also be similarly approximated. Then, given suitable boundary conditions in terms of u or its derivatives (i.e. stress), solutions of Navier's three equations proceed by repeatedly sweeping over the discretized grid and iteratively solving what amounts to a large, coupled set of algebraic equations. Some approaches to iteration are referred to as "relaxation" schemes and are related in some ways to the minimization principles which we will introduce in the next Methods section. These and other basic ideas are more fully expounded in some of the previous references; an additional reference that is a particular classic for analytic solutions in continuum mechanics as well as serving as an introduction to the numerical methods above is:

*Theory of Elasticity b*y Timoshenko and Goodier, Appendix, McGraw-Hill, 3rd edn, 1970.