

THE TRANSITION FROM PARTICLE DYNAMICS TO CONTINUUM MECHANICS

Consider a single particle of mass m , constrained to linear motion along the x -axis. If we denote its position at time t by $x(t)$ and if it moves in a field of force with potential $V(x,t)$, then its motion is described by Newton's second law

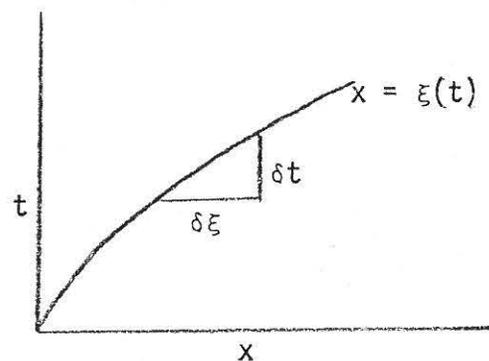
$$m \frac{d^2x}{dt^2} = - \frac{\partial V(x,t)}{\partial x} \quad (1)$$

This is the customary way of writing the second law, but it is confusing since x is simultaneously a dependent and an independent variable. It is less confusing to state that the particle path is some function $\xi(t)$ and that the force is evaluated at the point $x = \xi(t)$. Thus Eq. (1) becomes

$$\frac{d^2\xi}{dt^2} = - \left[\frac{\partial V(x,t)}{\partial x} \right]_{x = \xi(t)} \quad (2)$$

The meaning of the partial derivative in Eq. (2) is simple and clear: it represents the rate of change of V with respect to x while t is fixed; i.e., at a particular instant of time. The block derivative, d/dt , represents the rate of change experienced or recorded by an observer moving with the particle. This is best illustrated by drawing a graph of particle path in the (x,t) plane.

The limit of $\delta\xi/\delta t$ as $\delta t \rightarrow 0$ is $d\xi/dt$; neither x nor t is held constant. The distinction between this derivative and the partial derivative with x or t held constant is very important. Understanding it is essential to understanding the Lagrange and Euler coordinate representations of the flow equations.



Now suppose that a stream of particles is issuing into the force field from a slit at $x = 0$. To distinguish one particle from another we label them with the time they issue from the slit: particle "1" emerges at t_1 and follows

a path $\xi(t_1, t)$, "2" emerges at t_2 and has path $\xi(t_2, t)$, . . ., "j" emerges at t_j and follows $\xi(t_j, t)$. Then Eq. (2) becomes, for the j^{th} particle

$$m_j \frac{\partial^2 \xi(t_j, t)}{\partial t^2} = - \left[\frac{\partial V(x, t)}{\partial x} \right]_{x = \xi(t_j, t)} \quad (3)$$

The partial derivative on the left indicates that t_j is held constant; i.e., Eq. (3) applies to the j^{th} particle. Velocity, $u(t_j, t)$, now becomes a field variable, depending on t_j and t :

$$u(t_j, t) = \left[\partial \xi(t_j, t) / \partial t \right]_{t_j} \quad (4)$$

Equation (3) has mixed character. There are three independent variables, t , t_j , x , but two should suffice. t_j can be readily converted to a space variable; to do so, multiply it by the velocity with which the j^{th} particle issues from the slit:

$$y_j \equiv u_0^j t_j$$

If the distance between particles is very small, it is possible to reduce the number of independent variables in Eq. (3) if x is replaced by y_j . The particle label, t_j or y_j , is called a Lagrange coordinate. It can be replaced by other, equivalent labels. One common choice is to suppose that the stream of particle extends to $x = -\infty$ and to take the position of each particle at a particular time, say $t = 0$, as the Lagrange coordinate. Call this position $x_0(j)$. Then $\xi(x_0, t)$ is the position at time t of the particle which was at x_0 at $t = 0$, $x_0 = \xi(x_0, 0)$. Equation (3) becomes

$$m(x_0) \frac{\partial^2 \xi(x_0, t)}{\partial t^2} = - \left[\frac{\partial V(x, t)}{\partial x} \right]_{x = \xi(x_0, t)} \quad (5)$$

If particles are so numerous that many of them lie within a small increment of distance dx_0 , we have the possibility of replacing the space coordinate, x , on the r.h.s. of Eq. (5) by the Lagrange space coordinate, x_0 . Let $\xi(x_0(j), t)$ be the position of the j^{th} particle at time t and $\xi(x_0(k), t)$ be the position of the k^{th} particle at time t , where $x_0(k) = x_0(j) + dx_0$. Then

$$\xi(x_0(k), t) - \xi(x_0(j), t) = d\xi = \left. \frac{\partial \xi}{\partial x_0} \right|_t dx_0$$

Since we are now dealing with many closely spaced particles, $d\xi$ at fixed t is equal to dx , and the r.h.s. of Eq. (5) has the same meaning as

$$\left(\frac{\partial V(\xi, t)}{\partial \xi} \right)_t .$$

If we define $V'(x_0, t) \equiv V(\xi, t)$,

$$\begin{aligned} \partial V(\xi, t) / \partial \xi &= [\partial V'(x_0, t) / \partial x]_t \\ &= \frac{\partial V'}{\partial x_0} \Big|_t \frac{\partial x_0}{\partial \xi} \Big|_t \end{aligned}$$

where $(\partial x_0 / \partial \xi)_t = 1 / (\partial \xi / \partial x_0)_t$ as defined above. Now Eq. (5) becomes

$$m(x_0) \frac{\partial^2 \xi(x_0, t)}{\partial t^2} = - \frac{\partial V'}{\partial x_0} \frac{\partial x_0}{\partial \xi} \quad (6)$$

In these circumstances we may not be interested in single particles, but rather in groups of particles, say in the group with labels lying between x_0 and $x_0 + dx_0$. If the density of particles, i.e. number per unit length, is $n(x_0, 0)$ at $t = 0$ then the mass between x_0 and $x_0 + dx_0$ is $n(x_0, 0) dx_0 m(x_0)$. Summing Eq. (6) over this group of particles gives

$$n_0 m(x_0) dx_0 \left(\frac{\partial^2 \xi(x_0, t)}{\partial t^2} \right)_{x_0} = - \frac{\partial V'}{\partial x_0} \frac{\partial x_0}{\partial \xi} n(x_0) dx_0 \quad (7)$$

where $n_0 \equiv n(x_0, 0)$.

(Note that $n(x_0, t) \equiv n(x_0, 0)$; since the label attached to a particle is always the same, the number of particles between two labels is fixed and the separation, dx_0 , between two labels is also fixed.)

If we define mass per unit length at $t = 0$ as $\rho_0(x_0) = n_0 m(x_0)$ and factor dx_0 from Eq. (7), we have the equation of motion of a stream of non-interacting particles in Lagrange coordinates:

$$\rho_0 \frac{\partial^2 \xi}{\partial t^2} = - \rho_0 \frac{\partial V'}{\partial x_0} \frac{\partial x_0}{\partial \xi} . \quad (8)$$

When particles become densely packed, they will certainly interact. Let the potential of interaction between particles j and k be

$$\phi(\xi_j - \xi_k) = \phi[\xi(x_0^j, t) - \xi(x_0^k, t)]$$

ϕ is repulsive at small separation and attractive but rapidly diminishing in value at large separations. For example, a frequently used potential is of the "six-twelve" type:

$$\phi(r) = -a/r^6 + b/r^{12}.$$

The force on particle j resulting from the presence of particle k is

$$F_{jk} = -\partial\phi/\partial\xi_j.$$

Similarly, that on k due to j is

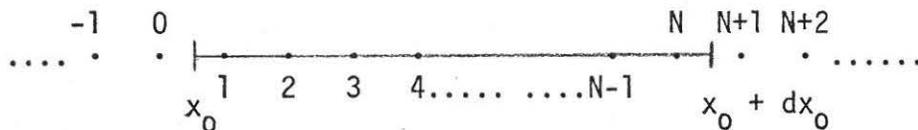
$$F_{kj} = -\partial\phi/\partial\xi_k = \partial\phi/\partial\xi_j = -F_{jk}. \quad (9)$$

Taking these forces of interaction into account, Eq. (6) for the j^{th} particle becomes

$$m_j \frac{\partial^2 \xi_j}{\partial t^2} = - \frac{\partial V'}{\partial x_0} \frac{\partial x_0}{\partial \xi} + \sum_{k=-\infty}^{\infty} F_{jk} \quad (10)$$

where the sum over k is taken over all atoms except j .

Next consider all the particles lying between x_0 and $x_0 + dx_0$. There are, on the average $n_0 dx_0$ such particles. Label them 1, 2, . . . , $N = n_0 dx_0$ in order of their increasing values of x_0 ; thus:



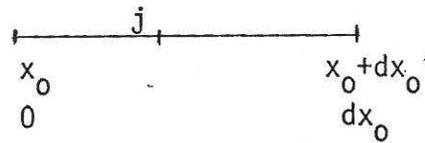
Since we are interested in finding the collective equation of motion of all the particles in dx_0 , we sum Eq. (10) for $j = 1$ to N :

$$dx_0 \rho_0 \frac{\partial^2 \xi(x_0, t)}{\partial t^2} = - n_0 \frac{\partial V'}{\partial x_0} \frac{\partial x_0}{\partial \xi} dx_0 + \sum_{j=1}^N \sum_{k=-\infty}^{\infty} F_{jk} \quad (11)$$

The sum over k can be written in three parts, giving

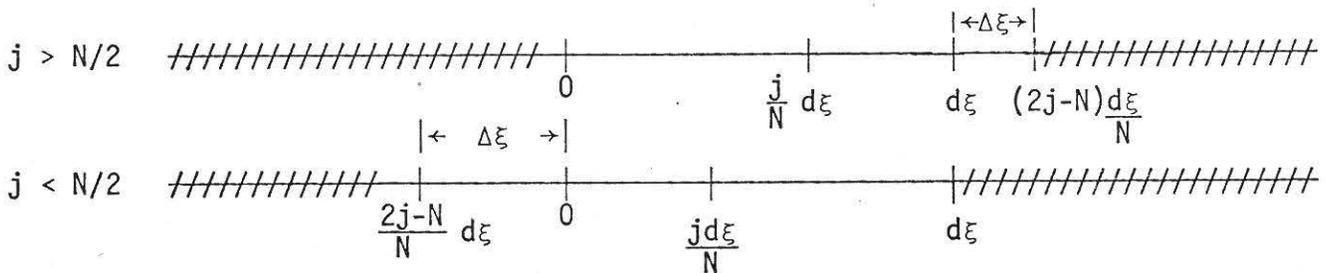
$$\sum_{j=1}^N \sum_{k=-\infty}^{\infty} F_{jk} = \sum_{j=1}^N \sum_{k=-\infty}^0 F_{jk} + \sum_{j=1}^N \sum_{k=1}^N F_{jk} + \sum_{j=1}^N \sum_{k=N+1}^{\infty} F_{jk} \quad (12)$$

The middle term is identically zero since $F_{jk} = -F_{kj}$. This is expected since internal forces cannot influence the motion of the center of mass of a system. Of the remaining two terms, the first represents force acting on the mass element $n_0 m dx_0$ due to the presence of atoms to the left of x_0 ; the second represents force due to atoms to the right of $x_0 + dx_0$. Consider now the force acting on a particular particle, say j , which lies within dx_0 . Choose the origin of coordinates at x_0 to simplify the notation. If the density of particles



in ξ -coordinates changes negligibly in a distance equal to the "range" of the potential ϕ , then the forces

due to groups of particles symmetrically disposed about particle j will cancel on the average and the net force acting on j is due to a small group of atoms lying within a distance $\Delta\xi$ of the boundaries of the interval $d\xi$ within which particle j is situated. This is illustrated in the following sketches. The cross-hatched intervals produce forces which cancel, and the net force on j is

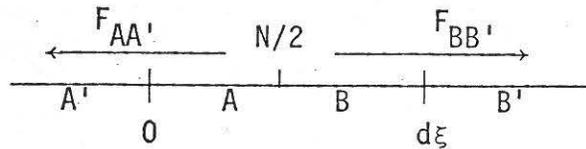


due to those particles within the interval $\Delta\xi$:

$$j < \frac{N}{2} \quad F_j = \sum_{k=-\frac{\Delta\xi}{n_0} \frac{\partial \xi}{\partial x_0}}^0 F_{jk} \quad F_{jk} = \sum_{k=2j-N}^0 F_{jk}$$

$$j > \frac{N}{2} \quad F_j = \sum_{k=N+1}^{N+\frac{\Delta\xi}{n_0} \frac{\partial \xi}{\partial x_0}} F_{jk} \quad F_{jk} = \sum_{k=N+1}^{2j-N} F_{jk}$$

Still under the assumption of uniform density, we see that by summing over all j , the net force on the mass between 0 and $d\xi$ vanishes. For every particle in A with $j < N/2$, there is, on the average, a particle symmetric about the midpoint $N/2$.



For every particle A' acting on A from the left, there is a symmetric particle B' acting on B from the right. $F_{BB'} = -F_{AA'}$, so by summing over j we find the net force vanishes. In order that there be a net average force, the number density, $n(\xi)$ must vary with ξ .

To estimate interaction forces on the particles contained within ξ is very difficult for an arbitrary potential ϕ . We can, however, introduce the macroscopic concept of stress or tension at this point and obtain the usual continuum approximation.



The force, F^- , acting on all of the particles to the left of the element $d\xi$ is equivalent to a tension T acting on that boundary. If the range of the interaction force, F_{jk} , is less than $d\xi$, the particles to the right of $d\xi$ contribute nothing to $F^- = T$, so we can now consider the element $d\xi$ isolated from the rest of the particles, whose influence is replaced by a force T on the left boundary and a second force, $T + \frac{\partial T}{\partial \xi} d\xi$ on the right boundary.



Then the net force acting on $d\xi$ is $\frac{\partial T}{\partial \xi} d\xi$, and this may be included on the r.h.s. of Eq. (11) to represent the double sum written there. Then the equation of motion is

$$\rho_0 \frac{\partial^2 \xi(x_0, t)}{\partial t^2} = -n_0 \frac{\partial V'}{\partial x_0} \frac{\partial x_0}{\partial \xi} + \frac{\partial T}{\partial \xi} \frac{\partial \xi}{\partial x_0} \quad (13)$$

What we have called the tension T may also be called the stress, σ , or the negative of the pressure, $T \rightarrow -p$, depending on the problem. While we have considered explicitly a linear stream of particles, the same ideas apply to the dynamics of continuous motion in a fluid or solid, extending to three dimensions. If the motion depends on only one Cartesian space coordinate, Eq. (13) applies with the appropriate interpretation of T . The potential most often considered is gravitational and proportional to the particle mass. Then $V' = m\Omega$ and Eq. (13) becomes

$$\frac{\partial^2 \xi(x_0, t)}{\partial t^2} = - \frac{\partial \Omega}{\partial x_0} \frac{\partial x_0}{\partial \xi} + \frac{1}{\rho_0} \frac{\partial T}{\partial \xi} \frac{\partial \xi}{\partial x_0} \quad (14)$$

Euler coordinates

We have taken care to write Eq. (14) in terms of x_0 and t and to define $\xi(x_0, t)$ as the position on the x axis, at time t , of the mass element initially at x_0 . The x -coordinate, fixed in the laboratory, is an Eulerian space coordinate. We can write Eq. (14) in Eulerian coordinates in the following way. Let $u \equiv (\partial \xi / \partial t)_{x_0}$ be the particle velocity, i.e., the rate at which a mass element is travelling along the x -axis.

If we look at all points on the x -axis simultaneously, we find that u varies from point to point, i.e., u is a function of (x, t) , say $u = u'(x, t)$. Then

$$\left[\frac{\partial u'(x, t)}{\partial t} \right]_{x_0} = \left(\frac{\partial u'}{\partial t} \right)_x + \left(\frac{\partial u'}{\partial x} \right)_t \left(\frac{\partial x}{\partial t} \right)_{x_0}$$

But $(\partial x / \partial t)_{x_0}$ is the same as $(\partial \xi / \partial t)_{x_0}$ [see the x - t diagram in which $\xi(t)$ is plotted], so that

$$\left(\frac{\partial u'}{\partial t} \right)_{x_0} = \left(\frac{\partial u'}{\partial t} \right)_x + u \left(\frac{\partial u'}{\partial x} \right)_t .$$

Since $u \equiv u'$, this is the same as

$$\left(\frac{\partial u}{\partial t} \right)_{x_0} = \left(\frac{\partial u}{\partial t} \right)_x + u \left(\frac{\partial u}{\partial x} \right)_t \equiv \frac{du}{dt} \quad (15)$$

$\frac{du}{dt}$ is defined by this relation. It is often called the convective derivative of u with respect to t .

We earlier determined a relation between dx_0 and $d\xi$:

$$d\xi = \frac{\partial \xi}{\partial x_0} dx_0$$

replacing $d\xi$ by dx and substituting this and (15) into Eq. (14) gives the equation of motion in Euler coordinates:

$$\frac{du}{dt} = - \frac{\partial \Omega}{\partial x} + \frac{1}{\rho} \frac{\partial T}{\partial x} \quad (16)$$

We have already stated the conservation of mass in the form

$$\rho_0 dx_0 = \rho d\xi$$

$$\text{or} \quad \rho_0 / \rho = (\partial \xi / \partial x_0)_t \equiv (\partial x / \partial x_0)_t \quad (17)$$

To express this in Eulerian coordinates, differentiate with respect to t at constant x_0 :

$$- \frac{\rho_0}{\rho^2} \left(\frac{\partial \rho}{\partial t} \right)_{x_0} = \frac{\partial^2 \xi}{\partial x_0 \partial t} = \frac{\partial u}{\partial x_0}$$

Applying Eq. (17) again, this becomes

$$- \frac{\rho_0}{\rho^2} \frac{d\rho}{dt} = \frac{\rho_0}{\rho} \frac{\partial u}{\partial x_0} \quad (18)$$

The equation for conservation of energy is just the First Law:

$$\frac{dE}{dt} = \frac{dQ}{dt} + \frac{dW}{dt} \quad (19)$$

where dW/dt is the rate of doing work on a mass element.