Energy Functionals in Mechanics

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Spring 2024

1 Lagrangian and Weak Form

Hamilton's Principle states that the dynamics of a system are governed by a stationary point of the Lagrangian, an energy functional defined as

$$\mathcal{L} := \int_0^T T - V dt$$

where T is the kinetic energy and V is the potential energy. This is core to classical mechanics, and is sometimes referred to as the "principle of least action." When minimization principles arise in physics, it is often tempting to become philosophical and read a kind of parsimony into nature, saying that among all possible events, those which unfold are optimal in some sense. I have explored elsewhere that Hamilton's Principle is not actually a minimization principle. Rather, dynamics of a system are governed by a *stationary point* of the Lagrangian, which in many realistic situations is a saddle point. The Lagrangian often seems like a mysterious thing. Here, we can demystify it by showing that it is arises naturally from a set of governing equations which are based on Newton's second law. The same derivation can be conducted for other systems governed by $F = ma$. The takeaway is this: *the Lagrangian is recognized as a functional whose stationary points correspond to the weak form of the governing equations.* I view the strong form of the governing equations as the most "real" in the sense that they are closest to the fundamental physical law of the balance of linear momentum. For solid mechanics, which we will explore here, they are a direct statement of this law. Newton's laws are the empirical content of mechanics. The rest is just math, or at least this is what I think. It turns out that formulating energy functionals tends to be very *convenient* in practice, but I think we should be hesitant to read too much into them. The equations of motion for an elastic solid are

$$\rho \ddot{u}_i = \frac{\partial \sigma_{ij}}{\partial x_j} + b_i$$

For linear elasticity, we have that $\sigma_{ij} = C_{ijk\ell}\epsilon_{k\ell} = C_{ijk\ell}\frac{\partial u_k}{\partial x_\ell}$. Here, we make use of the strain-displacement relation and symmetries of the constitutive tensor. We compute a space-time weak solution of the governing equations

by integrating against a test function $w_i(x,t)$. This contrasts with a common approach to weakening time-dependent problems where the time dimension is not integrated. The space-time weak form for linear elasticity is

$$\int_0^T \int_\Omega \rho \ddot{u}_i w_i(x,t) d\Omega dt = \int_0^T \int_\Omega \frac{\partial}{\partial x_j} C_{ijk\ell} \frac{\partial u_k}{\partial x_\ell} w_i(x,t) + b_i w_i(x,t) d\Omega dt$$

The spatial integral is taken over the volume of the elastic body, and the time integral is taken up to an arbitrary final time T. We can integrate the spatial derivative in the stress term onto the test function, and one time derivative from the acceleration onto the test function. Note that the boundary term from the spatial derivatives exposes the traction boundary condition. This expression becomes

$$-\int_0^T \int_\Omega \rho \dot{u}_i \dot{w}_i d\Omega dt = -\int_0^T \int_\Omega C_{ijk\ell} \frac{\partial u_k}{\partial x_\ell} \frac{\partial w_i}{\partial x_j} d\Omega dt + \int_0^T \int_{\partial\Omega} t_i w_i dS dt + \int_0^T \int_\Omega b_i w_i d\Omega dt$$

Why is there no boundary term in the time integration? We have an initial condition $u(x,0) = u_0$ which ensures that $w(x,0) = 0$. In other words, the test function is zero where the solution is prescribed. Why is it also zero at the final time? I think the intuition is that the second initial condition, which prescribes the velocity of the solution at the initial time, uniquely prescribes the solution at the final time, thus we think of this as also known. Regardless of the reason, the assumption of zero variation at the final time is standard calculus of variations trickery that simplifies the problem. The above expression is the space-time weak form of the equations of motion for a linearly elastic solid. We now recognize this equation as a condition for a stationary point of an energy functional defined as

$$\mathcal{L} := \int_0^T \int_\Omega \frac{1}{2} \rho \dot{u}_i \dot{u}_i - \frac{1}{2} C_{ijk\ell} \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_\ell} + b_i u_i d\Omega dt + \int_0^T \int_{\partial\Omega} t_i u_i dS dt$$

where w_i is the variation. Using the symmetries of the constitutive tensor and the strain-displacement relations, we can recognize that second term in the integral as the strain energy density:

$$\Psi := \frac{1}{2} C_{ijk\ell} \epsilon_{ij} \epsilon_{k\ell}$$

The first term is the kinetic energy. The third and fourth terms are the work performed by volumetric forces and surface tractions respectively. This is the Lagrangian. We recover the weak form of the equations of motion by computing the condition of stationarity with the calculus of variations. This is often written as

$$\delta \mathcal{L} = 0$$

The test function from the weak form is recognized as a variation when a variational principle of this sort exists. Note that when treating a statics problem, there is no time dependence on the solution. Thus, the kinetic energy is zero, and the time integration is trivial. The energy functional for the static problem is

$$\Pi := \int_\Omega \Psi - b_i u_i d\Omega - \int_{\partial\Omega} t_i u_i dS$$

where the factor of T is omitted because the stationary point of a functional does not change with multiplicative scaling. To be clear, the surface integral is only taken over regions where the traction is prescribed, which may not be the whole boundary. In solid mechanics, this energy functional is often called the "total potential energy." The strain energy term is called the internal potential, and the work terms are called the external potential. Their sum is thus deemed a total potential. We can show that a stationary point of the total potential is in fact a minimum by taking the second variation. It can be seen that

$$\delta^2\Pi = \delta\left(\int \frac{\partial\Psi}{\partial\epsilon_{ij}}\frac{\partial w_i}{\partial x_j} - b_i w_i d\Omega - \int t_i w_i dS\right) = \int \frac{\partial^2\Psi}{\partial\epsilon_{ij}\partial\epsilon_{k\ell}}\frac{\partial w_i}{\partial x_j}\frac{\partial w_k}{\partial x_\ell}d\Omega$$

The variations w are arbitrary. The condition for the stationary point to be a minimum is that the second variation (generalization of the second derivative) is positive. Under what conditions is the integral in the above expression guaranteed to be greater than zero? The requirement here is that

$$\frac{\partial^2\Psi}{\partial\epsilon_{ij}\partial\epsilon_{k\ell}} \quad = \quad \text{positive definite}$$

For linear elasticity, the second strain derivative of the energy is the constant constitutive tensor $C_{ijk\ell}$ which is in fact positive definite. Thus, stationary points of the total potential energy are minima, and their uniqueness is also a property of the positive definite-ness of the constitutive tensor. This is not the case for dynamics.

The final question we might ask is: is there any clear sense in which this functional is truly some *total* energy? To investigate this, we can state the so-called "Clapeyron theorem," which quantifies the exchange of energy in the elastic deformation. We start with the total elastic energy stored in the body, which is written simply as

$$\int_\Omega \Psi d\Omega = \int_\Omega \frac{1}{2}\sigma_{ij}\epsilon_{ij}d\Omega = \int_\Omega \frac{1}{2}\sigma_{ij}\frac{\partial u_i}{\partial x_j}d\Omega$$

The last step follows from the strain-displacement relations and the symmetry of the stress tensor. We can use integration by parts to write this as

$$= -\frac{1}{2}\int_\Omega \frac{\partial \sigma_{ij}}{\partial x_j} u_i d\Omega + \frac{1}{2}\int_{\partial\Omega} \sigma_{ij} u_i n_j dS = \frac{1}{2}\int_\Omega b_i u_i d\Omega + \frac{1}{2}\int_{\partial\Omega} t_i u_i dS$$

The last step follows from using the equilibrium equations and the definition of a traction vector on a surface. What this shows is that the total strain energy stored in the body equals the work done by quasi-statically applied external forces. The factor of $\frac{1}{2}$ comes from the quasi-static assumption, which says that the force and displacement are linearly dependent on one another. In other words, the work done by the traction forces going from a displacement of 0 to u^* is

$$W_{trac} = \int_{\partial\Omega}\int_0^{u^*} t(\xi)\xi d\xi dS$$

where because of the linearity of the material, we assume that the relationship $t(\xi)$ is linear. This relationship, which says that the internal energy is equal to the work done by quasi-statically applied external forces, might make you think twice about whether the total potential energy has any physical meaning. While its interpretation is not totally clear, what is clear is that its minimum corresponds to a solution to the elasticity problem.

2 A General Variational Form

Differential equations which correspond to stationary points of energy functionals are always interesting. When such a formulation exists, the energy can be discretized and then extremized. Well known energy functionals in mechanics are the Lagrangian from classical mechanics and the total potential energy from solid mechanics. There are also canonical problems in the calculus of variations such as the catenary. This is the shape of a cable of fixed length hanging between two points. By giving the cable a mass per length, its shape can be found by minimizing its gravitational potential energy. That the cable has fixed length is introduced as a constraint using Lagrange multipliers. This problem is classic and interesting enough to deserve a brief investigation. Call the mass per unit length μ. The total potential energy of the cable is

$$V = \int_0^L \mu g y ds, \quad y(0) = y_0, \quad y(L) = y_1$$

where g is the gravitational constant, L is the space between supports, y is the height at each point, and ds is the arc-length of the cable. The heights at either end are the supports of the cable and are prescribed. We will write the vertical height in terms of the horizontal position x, and use the expression for a differential arc length to write this as

$$V\Big(y(x)\Big) = \int_0^L \mu g y \sqrt{1 + \left(\frac{\partial y}{\partial x}\right)^2} dx$$

Now, we introduce the constraint that the cable has a fixed length ℓ. This is simply

$$G\Big(y(x)\Big) = \int_0^L \sqrt{1 + \left(\frac{\partial y}{\partial x}\right)^2}\, dx = \ell$$

We use Lagrange multipliers to enforce this constraint while minimizing the potential energy V. The common situation for Lagrange multipliers is that a constraint $g = 0$ is multiplied by an unknown Lagrange multiplier λ and added to the energy function or functional. This is what you will encounter on wikipedia or most other sources on the topic. However, when presenting the catenary derivation, the constraint $G = \ell$ is used instead of $G - \ell = 0$. See for yourself at sites like this one. This seems to be some kind of trick which lends itself to an analytical treatment of this problem. We are not too concerned with being able to solve problems analytically, and thus stick with the usual approach. The constrained energy functional is then

$$\mathcal{L}\Big(y(x), \lambda\Big) = \int_0^L \mu g y \sqrt{1 + \left(\frac{\partial y}{\partial x}\right)^2}\, dx + \lambda\left(\int_0^L \sqrt{1 + \left(\frac{\partial y}{\partial x}\right)^2}\, dx - \ell\right)$$

It can be shown that extrema of functionals constrained by Lagrange multipliers are saddle points, taking a maximum over λ and a minimum over the solution field. The first step in obtaining a solution is to discretize the height function with

$$y(x) = y_0 + \left(\frac{y_1 - y_0}{L}\right)x + \sum_i a_i f_i(x)$$

where the first term enforces the boundary conditions, and shape functions respect the boundaries with $f_i(0) = f_i(L) = 0$. We can plug in this discretization, and write the Lagrangian abstractly as

$$\mathcal{L}\Big(\underline{a}, \lambda\Big) = F(\underline{a}) + \lambda\Big(G(\underline{a}) - \ell\Big)$$

The condition for a stationary point is then

$$\frac{\partial \mathcal{L}}{\partial a_i} = \frac{\partial F}{\partial a_i} - \lambda \frac{\partial G}{\partial a_i} = 0$$
$$\frac{\partial \mathcal{L}}{\partial \lambda} = G(\underline{a}) - \ell = 0$$

This is a nonlinear system of equations that can be solved with a Newton-Raphson method. The coefficients and Lagrange multiplier are updated iteratively with

$$\begin{bmatrix} \Delta \underline{a}^k \\ \Delta \lambda^k \end{bmatrix} = -\begin{bmatrix} \frac{\partial^2 \mathcal{L}}{\partial \underline{a} \partial \underline{a}} & \frac{\partial^2 \mathcal{L}}{\partial \underline{a} \partial \lambda} \\ \frac{\partial^2 \mathcal{L}}{\partial \lambda \partial \underline{a}} & \frac{\partial^2 \mathcal{L}}{\partial \lambda \partial \lambda} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial \mathcal{L}}{\partial \underline{a}} \\ \frac{\partial \mathcal{L}}{\partial \lambda} \end{bmatrix}$$

$$\begin{bmatrix} \Delta \underline{a}^{k+1} \\ \Delta \lambda^{k+1} \end{bmatrix} = \begin{bmatrix} \underline{a}^{k} \\ \lambda^{k} \end{bmatrix} + \begin{bmatrix} \Delta \underline{a}^{k} \\ \Delta \lambda^{k} \end{bmatrix}$$

It is nice to stay closer to the usual Lagrange multipliers with this method, and it is interesting to solve canonical problems from the calculus of variations in a "computational" way.

This was a bit of a detour before presenting a general variational form which can be used to generate a whole class of equations. Consider the following energy-like functional:

$$I\Big(u(x)\Big) = \int_\Omega \left(\int_0^{|\nabla u|} \rho(s) s ds + \int_0^u h(s) ds \right) d\Omega$$

The condition for stationarity is

$$\delta I = 0 = \int_\Omega \left(\rho(|\nabla u|) |\nabla u| \frac{\partial |\nabla u|}{\partial \left(\frac{\partial u}{\partial x_i} \right)} \frac{\partial \delta u}{\partial x_i} + h(u) \delta u \right) d\Omega$$

It can be shown in index notation that

$$\frac{\partial |\nabla u|}{\partial \left(\frac{\partial u}{\partial x_i} \right)} = \frac{1}{|\nabla u|} \frac{\partial u}{\partial x_i}$$

which means that the above expression becomes

$$0 = \int_\Omega \rho(|\nabla u|) \frac{\partial u}{\partial x_i} \frac{\partial \delta u}{\partial x_i} + h(u) \delta u d\Omega$$

The strong form of the governing equations is obtained through integration by parts and noting that the variation is arbitrary. This reads

$$\frac{\partial}{\partial x_i} \left(\rho(|\nabla u|) \frac{\partial u}{\partial x_i} \right) - h(u) = 0$$

Thus we can construct variational principles for strong form governing equations where the displacement-like variable u shows up in arbitrary nonlinear ways. With this approach, there are more restrictions on the form of the derivatives. It is not simple to find a variational principle corresponding to arbitrary combinations of derivatives. It also difficult and sometimes provably impossible to construct variational principles for mixed terms of the form $u \frac{\partial u}{\partial x}$. This is the situation for the advection term in fluid mechanics, for example. The above equation could be used to find an energy functional for radiative heat transfer, which is governed by a u^4 source term, where the thermal conductivity depended on the temperature gradient. To be fair, it seems that gradient-dependence of the conductivity is much less physical than temperature-dependence. It is perhaps interesting to note that we can obtain the Helmholtz equation from this method with $\rho(|\nabla u|) = -1$ and $h(u) = u$. In this case, the energy is

$$I\Big(u(x)\Big) = \int_\Omega \frac{1}{2}\frac{\partial u}{\partial x_i}\frac{\partial u}{\partial x_i} - \frac{k}{2}u^2 d\Omega$$

and the strong form of the governing equations are

$$\frac{\partial^2 u}{\partial x_i \partial x_i} + ku = 0$$

where k is the eigenvalue. Note that Helmholtz equation is an eigenvalue problem for the Laplace operator. It arises when using separation of variables to solve the wave equation. To see this, note that a generic wave equation is

$$\frac{\partial^2 U}{\partial t^2} = \nabla^2 U$$

In separation of variables, we assume a multiplicative decomposition of the solution $U = T(t)u(x, y)$. Plugging this into the governing equation, we obtain

$$u\frac{\partial^2 T}{\partial t^2} = T\nabla^2 u \implies \frac{\ddot{T}}{T} = \frac{\nabla^2 u}{u}$$

We use the usual trick to say that if two functions which each depend on different variables are equal to one another, they must be constant. We call this constant $-k$, and arrive at

$$\frac{\partial^2 T}{\partial t^2} = -kT$$

$$\nabla^2 u + ku = 0$$

The first equation shows that the temporal part of the solution consists of sines and cosines, whose second derivatives are negatives of themselves. Solving the spatial eigenvalue problem computationally should be quite easy. We take the Helmholtz equation and weaken it with a spatial test function w:

$$\int \nabla^2 u w d\Omega + k \int u w d\Omega = 0$$

We can integrate by parts and assume zero Neumann boundary conditions to obtain

$$\int \nabla u \cdot \nabla w d\Omega = k \int u w d\Omega$$

Discretizing both the test and trial functions with the same set of spatial shape functions multiplied by unknown degrees of freedom a_i leads to

$$K_{ij} a_j = k F_{ij} a_j$$

This is a standard generalized eigenvalue problem which can be solved for eigenvectors and their corresponding eigenvalues.