Lecture 3: Introduction to Analytical Mechanics

- Variational approach: presenting differential equations as an optimization problem
- Principles of analytical mechanics:
  - D'Alembert principle (virtual work)
  - Hamiltonian principle (stationary action)
- Generalized coordinates
  - Also the corresponding generalized forces, momenta, energy
- Lagrangian and pseudo-potential (dissipation function)
- Euler-Lagrange equations
- Conservation laws
- Spatially-dependent variables (fields)

- Reading: Chapters 3 and 4 in the text

Mechanics

- In classical mechanics, a system of any complexity is described as a collection of point masses m_k located at points $\mathbf{x}_k$. Force vectors $\mathbf{F}_k$ are applied to these masses
- Under the action of these forces, the acceleration of each mass equals (second Newton's law)

$$\mathbf{a}_k = \ddot{\mathbf{x}}_k = \frac{\mathbf{F}_k}{m_k}$$

Notation: $\ddot{\mathbf{x}}_k \overset{\text{def}}{=} \frac{\partial^2 \mathbf{x}_k}{\partial t^2}$

- This gives a (possibly large) number of equations for vectors $\mathbf{x}_k(t)$ for N_p particles. The forms of these equations change if we use, for example, spherical or cylindrical coordinates instead of Cartesian ones, etc.

- How to write all these equations in just one equation, and independently of the specific selection of the coordinate system?
- The answer is: use a variational principle. Formulations of mechanics based on mathematical variational principles are called analytical mechanics
  - Probably the best and most elegant one is based on "differential forms", but this may be too much for us

D'Alembert's principle

- To obtain a variational formulation, we need to first make an equation with the right-hand side equal zero:

$$m_k \ddot{\mathbf{x}}_k - \mathbf{F}_k = \mathbf{0}$$

  - This equation is sometimes called "conservation of momentum" in modeling literature, which I think is not a very good idea. There is no momentum here (yet).
  - More precisely, this equation simply means the balance of the external and inertial forces applied to each particle in its own frame of refence

- Now, let us perform arbitrary infinitesimal (called "virtual") perturbations of the trajectory of each particle:

$$\mathbf{x}'_k(t) = \mathbf{x}_k(t) + \delta\mathbf{x}_k(t)$$

- …and evaluate the virtual work of all of the above forces:

$$\delta W = \sum_{k=1}^{N_p} \left(m_k \ddot{\mathbf{x}}_k - \mathbf{F}_k \right) \delta\mathbf{x}_k = 0$$

- This is the d'Alembert principle: the correct trajectories $\mathbf{x}_k(t)$ are such that the total virtual work is stationary : $\delta W = 0$ for arbitrary perturbations $\delta\mathbf{x}_k(t)$

Hamiltonian principle

- The d'Alembert principle is called **quasi-variational**, because the virtual work δW is not a variation of any 'functional'
  - 'Functional' means a function (some real value) attributed to the whole collection of trajectories (functions) $\mathbf{x}_k(t)$ taken at all times
- To obtain a functional of trajectories $\mathbf{x}_k(t)$, we can integrate δW over time t and sum over all particles:

$$\delta S = \int_{t_1}^{t_2} \delta W dt = \int_{t_1}^{t_2} \sum_{k=1}^{N_p} \left(m_k \ddot{\mathbf{x}}_k - \mathbf{F}_k \right) \delta \mathbf{x}_k dt = 0$$

  - This summation gives a scalar function ('functional') of all trajectories $\mathbf{x}_k(t)$: $S\{\mathbf{x}_k(t)\}$
  - This functional S is called the Hamiltonian action
  - All Newton's equations of motion are then contained in the requirement that $\delta S = 0$ for an arbitrary perturbation of trajectories $\delta \mathbf{x}_k(t)$
- This is the **true variational** principle of stationary Hamiltonian action

Note that unlike the 'correspondence principle' in the viscoelastic model, this principle is not a phenomenological hypothesis but a very general form of Newton's laws

Lagrangian

- For each particle, the two terms in the variation of action are:

$$\int_{t_1}^{t_2} m_k \ddot{\mathbf{x}}_k \delta \mathbf{x}_k dt = \int_{t_1}^{t_2} \delta T_k dt \qquad \text{where} \qquad T_k = \frac{1}{2} m_k \dot{\mathbf{x}}_k^2 \qquad \text{is the kinetic energy}$$

and $\mathbf{F}_k \delta \mathbf{x}_k = -\delta U_k$, where U_k is the potential (elastic) energy

- Therefore,

$$S = \int_{t_1}^{t_2} L dt \qquad \text{where} \qquad L = \sum_{k=1}^{N_p} (T_k - U_k) \qquad \text{is called the Lagrangian function of the complete mechanical system}$$

- Therefore, for an arbitrary mechanical system, all equations of motion are contained in a single variational equation:

$$\delta S = \delta \left[\int_{t_1}^{t_2} L dt \right] = 0 \qquad \text{for arbitrary deviations } \delta \mathbf{x}_k(t) \text{ from the true trajectories}$$

Lagrangian

- The Lagrangian is usually the difference of the total kinetic and elastic energies: $L = \sum_{k=1}^{N_p} (T_k - U_k)$ but it does not have to be only that
- For example, for electric charges q_k in a magnetic field (nonconservative, forces are not gradients of a potential function), the corresponding part of the Lagrangian is

$$L_{mag} = \sum_{k=1}^{N_p} \left(-\frac{q_k}{c} \dot{\mathbf{x}}_k \mathbf{A} \right)$$

where $\mathbf{A}$ is the vector electromagnetic potential and c is the speed of light

$$\mathbf{B} = \nabla \times \mathbf{A}$$

Note that the Lagrangian depends on particle velocities instead of coordinates

- The Lagrangian can also be time-dependent
  - For example, in the presence of an external force $\mathbf{f}_k(t)$:

$$L_{ext} = \sum_{k=1}^{N_p} \mathbf{f}_k(t) \mathbf{x}_k$$

Dissipation function (pseudo-potential)

- In the variational approach, all elastic forces can be found by evaluating the perturbation of the elastic-energy part of the action. By making arbitrary infinitesimal perturbations of $\delta\mathbf{x}_k(t)$, the time integral of the elastic energy varies as

$$\delta\left[\int_{t_1}^{t_2} U dt\right] = -\sum_{k=1}^{N_p}\int_{t_1}^{t_2} \mathbf{F}_k \delta\mathbf{x}_k dt$$

This factor in front of $\delta\mathbf{x}$ (variational derivative) is the **force**

- Similarly, the forces of friction can be obtained by variation of another functional, but with respect to perturbations of velocities $\delta\dot{\mathbf{x}}_k$:

$$\delta\left[\int_{t_1}^{t_2} D dt\right] = -\sum_{k=1}^{N_p}\int_{t_1}^{t_2} \mathbf{F}_k \delta\dot{\mathbf{x}}_k dt$$

- The integrand D here is called the dissipation function, or pseudo-potential
- For example, if each of the bodies is a spherical particle of radius r_k moving through fluid with viscosity η, then it will experience a viscous friction force $\mathbf{F}_k = -6\pi r\eta\dot{\mathbf{x}}_k$ (Stokes' law), and the dissipation function for the system is:

$$D = 3\pi\eta\sum_{k=1}^{N_p} r_k \dot{\mathbf{x}}_k^2$$

Note that D often looks like kinetic energy

External forces and constraints

- Often, it is required that the system satisfies additional constraints
  - For example, such constraints can be boundary conditions at the free surface or open or closed conditions for pore-fluid flow across various boundaries
- Let us denote the constraint by equation $B_j\left(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \ldots\right) = 0$ (**)
- Then, we need to find the extremum of action

$$\delta S = \delta\left[\int_{t_1}^{t_2} L dt\right] = 0$$

not for arbitrary functions $\delta\mathbf{x}_k(t)$ but only for those satisfying eqs. (**). This can be done by adding constraint terms to the Lagrangian:

$$L \to L + \sum_{j=1}^{N_c} \lambda_j B_j$$

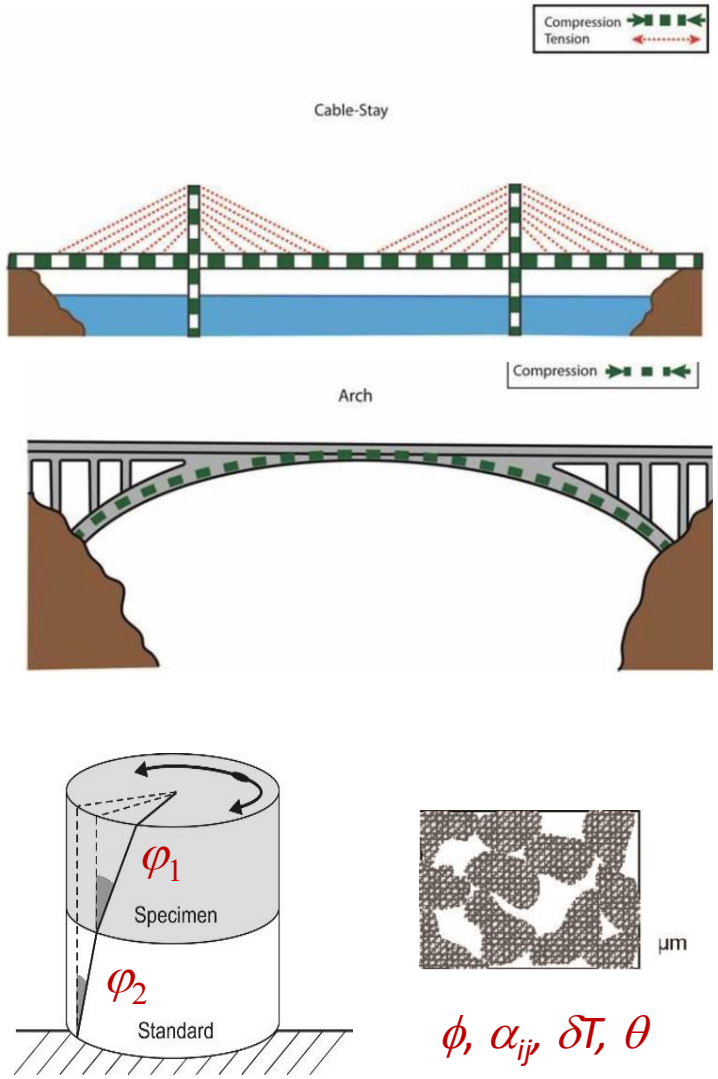
λ_j is called the Lagrange multiplier. It has the meaning of **external force** required to hold the variables at the constraint surface $B_j = 0$

- Then, variations of $\delta\mathbf{x}_k(t)$ can again be considered as arbitrary, and parameters λ_j selected to make the solution satisfy eqs. (**)

Generalized coordinates

- Up to this point, we used N_p particles with Cartesian coordinates $\mathbf{x}_k$ to describe the mechanical system (rock)
- However, the variational approach allows much broader parameterizations by arbitrary selections of generalized coordinates to describe the state of the system
  - The generalized coordinates should be some parameters which are the simplest, most sensitive, or most important for the goals of analysis
    - For example, the green or red elements of bridges undergoing compression and tension, or shearing angles of a rock sample on the right)
- The equation of stationary action is the same in any coordinates

$$\delta S = \delta\left[\int_{t_1}^{t_2} L dt\right] = 0$$



- The Lagrangian and dissipation function are functions of generalized coordinates $\mathbf{q}$ and their time derivatives $\dot{\mathbf{q}}$, and possibly time t:

$$L(t, \mathbf{q}, \dot{\mathbf{q}}) \quad \text{and} \quad D(t, \mathbf{q}, \dot{\mathbf{q}})$$

Euler-Lagrange equations

- In terms of the generalized variables, the perturbation of action $S = \int_{t_1}^{t_2} L dt$ equals (summation over repeated subscripts '$_i$' assumed)

$$\delta S = \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \right) dt$$

Transforming the second term by integration by parts, so that it contains δq_i this eq. becomes:

$$\delta S = \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right) \delta q_i dt = 0$$

- Therefore, for any i, $\mathbf{q}(t)$ must satisfy the Euler-Lagrange equation:

$$\frac{\delta S}{\delta q_i} = \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0$$

This expression is called the functional derivative of functional S with respect to function $q_i(t)$

- Adding forces of friction from dissipation function D, this equation becomes:

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} + \frac{\partial D}{\partial \dot{q}_i} = 0$$

Generalized momentum, forces, and energy

- The derivative $p_i = \dfrac{\partial L}{\partial \dot{q}_i}$

  is called the generalized momentum:
  - Regular momentum when q_i is a coordinate
  - Angular momentum when q_i is a rotation angle, etc.

- Similarly, the derivatives $Q_i = \dfrac{\partial L}{\partial q_i}$ and $R_i = -\dfrac{\partial D}{\partial \dot{q}_i}$ are generalized forces (conservative and dissipative
- Therefore, the Euler-Lagrange equations become just like second Newton's law:

$$\frac{dp_i}{dt} = Q_i + R_i$$

- Function $H = p_i \dot{q}_i - L$ (if p_i is expressed through $\mathbf{q}$ and $\dot{\mathbf{q}}$) is called the generalized energy (total mechanical energy of the system; again note the summation over repeated subscripts 'i')
  - Function H is also called the Hamiltonian if expressed through $\mathbf{p}$ and $\mathbf{q}$, or the Helmholtz free energy if adding effects of temperature

Conservation laws

- Conservation laws are obtained by noting the general properties of functions L and D:
  - Conservation of mechanical energy: If $D = 0$ and function *L* is explicitly independent of time, then the total mechanical energy H is conserved:

$$\frac{dH}{dt} = \frac{d}{dt}\left(p_i \dot{q}_i\right) - \frac{\partial L}{\partial q_i}\dot{q}_i - \frac{\partial L}{\partial \dot{q}_i}\ddot{q}_i = \frac{d}{dt}\left(p_i \dot{q}_i\right) - \dot{p}_i \dot{q}_i - p_i \ddot{q}_i \equiv 0$$

  - Conservation of momentum: If $D = 0$ and function L is explicitly independent of some q_i, then the corresponding momentum p_i is conserved:

$$\frac{dp_i}{dt} = Q_i = \frac{\partial L}{\partial q_i} = 0$$

- If $D \neq 0$, mechanical energy varies (dissipates) at rate

$$\frac{dH}{dt} = R_i \dot{q}_i = -\dot{q}_i \frac{\partial D}{\partial \dot{q}_i}$$

If function *D* is quadratic (as it usually is), this rate equals (-2D)

Spatially-dependent variables (fields)

- When modeling continuous media, variables q_i often represent functions of spatial coordinates $\mathbf{x}$. Therefore, in addition to $\mathbf{q}$ and time derivatives $\dot{\mathbf{q}}$, the Lagrangian and dissipation functions depend on the spatial derivatives of $\mathbf{q}$: $L\left(t, \mathbf{q}, \nabla\mathbf{q}, \dot{\mathbf{q}}, \nabla\dot{\mathbf{q}}\right)$
  - For example, this is the common case in the mechanics of solids: q_i is the components of spatially-variable displacement, and their spatial derivatives are the strain tensor
- Let us denote the spatial derivative with respect to coordinate x_j by comma in the subscript:

$$q_{i,j} = \frac{\partial q_i}{\partial x_j}$$

- Then, the Euler-Lagrange equations include additional spatial derivatives similar to the derivatives with respect to t:

$$\frac{\partial}{\partial t}\frac{\partial L}{\partial \dot{q}_i} + \frac{\partial}{\partial x_j}\frac{\partial L}{\partial q_{i,j}} - \frac{\partial L}{\partial q_i} + \frac{\partial D}{\partial \dot{q}_i} - \frac{\partial}{\partial x_j}\frac{\partial D}{\partial \dot{q}_{i,j}} = 0$$