An Introduction Hamiltonian Mechanics

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In this post I shall assume understanding of the concepts described in chapter 4 (Conservation of Energy), chapter 8 (Motion) as well as sections 11–4 and 11–5 (Vectors and Vector algebra) of chapter 11 of Richard Feynmann's *Lectures on Physics*.

It is the continuation of my *Introduction to Runge-Kutta Integrators*, but it does not rely on the concepts described in that post.

1 Motivation

We have previously seen how to compute the evolution of physical systems while keeping the buildup of error in check. However, the error will still build up over time. We would like to ensure that fundamental properties of the physical system are preserved. For instance, we'd like a low strongly-bound orbit not to turn into an escape trajectory (or a reentry) over time: we need conservation of energy.

In order to make an integrator that conserves energy, it is helpful to look at physics from a viewpoint where the conservation of energy is the fundamental hypothesis, rather than a consequence of the application of some forces.

2 Gravitation from a Hamiltonian viewpoint

We consider a system of N bodies 1 through N, with masses m_1 through m_j. The state of the system is defined by the *positions* and *momenta* of those bodies. For each body j, the position $\boldsymbol{Q}_j$ and the momentum $\boldsymbol{P}_j$ are 3-dimensional vectors, so the state of the entire system lies in a $6N$-dimensional space, the *classical*[1] *phase space*. We can write the state as $(\boldsymbol{q}, \boldsymbol{p})$, where $\boldsymbol{q} = (q_1, \dots, q_{3N})$ and $\boldsymbol{p} = (p_1, \dots, p_{3N})$ are $3N$-dimensional.

The total energy $\mathcal{H}$, the *Hamiltonian* is a function of the state of the system, the energy of a given state being $\mathcal{H}(\boldsymbol{q}, \boldsymbol{p})$.

The evolution of the state $(\boldsymbol{q}, \boldsymbol{p})$ is given for each component $i \in \{1, \dots, 3N\}$, by the *equations of motion*

$$\begin{cases} \frac{\mathrm{d}\,q_i}{\mathrm{d}\,t} &= \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,p_i} \\ \frac{\mathrm{d}\,p_i}{\mathrm{d}\,t} &= -\frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,q_i} \end{cases}.$$

This is can be written[2] as

$$\begin{cases} \frac{\mathrm{d}\,\boldsymbol{q}}{\mathrm{d}\,t} &= \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{p}} \\ \frac{\mathrm{d}\,\boldsymbol{p}}{\mathrm{d}\,t} &= -\frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{q}} \end{cases}.$$

In this way, we have *defined* the change in position and momentum as a function of time, and thus completely desccribed how the system will evolve from an initial state $(\boldsymbol{q}_0, \boldsymbol{p}_0)$.

[1] A similar formalism exists for quantum mechanics, in which case we talk about the *quantum* phase space.

[2] Readers familiar with multivariate calculus might prefer the notations $\frac{\mathrm{d}\,\boldsymbol{q}}{\mathrm{d}\,t} = \boldsymbol{\nabla}_{\boldsymbol{p}}\mathcal{H}$, $\frac{\mathrm{d}\,\boldsymbol{p}}{\mathrm{d}\,t} = -\boldsymbol{\nabla}_{\boldsymbol{q}}\mathcal{H}$, or $\frac{\mathrm{d}}{\mathrm{d}\,t}\begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{p}\end{pmatrix} = \begin{pmatrix}\boldsymbol{0} & \mathbb{1}\\ -\mathbb{1} & \boldsymbol{0}\end{pmatrix}\boldsymbol{\nabla}\mathcal{H}$.

From this formulation it immediately follows that energy is conserved: indeed,

$$\begin{aligned}\frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,t} &= \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{q}} \cdot \frac{\mathrm{d}\,\boldsymbol{q}}{\mathrm{d}\,t} + \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{p}} \cdot \frac{\mathrm{d}\,\boldsymbol{p}}{\mathrm{d}\,t} \\ &= \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{q}} \cdot \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{p}} - \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{p}} \cdot \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{q}} = 0.\end{aligned}$$

Here the energy is $\mathcal{H} = T + V$, where T is the kinetic energy and V is the gravitational potential energy. Since T only depends on the momenta $\boldsymbol{p}$ (recall that for body j, $T_j = \frac{1}{2} m_j v_j^2$ and $\boldsymbol{P}_j = m_j \boldsymbol{v}_j$) and V only depends on the positions $\boldsymbol{q}$, we get:

$$\mathcal{H}(\boldsymbol{p}, \boldsymbol{q}) = T(\boldsymbol{p}) + V(\boldsymbol{q})$$

so the equations of motion become

$$\begin{cases} \frac{\mathrm{d}\,\boldsymbol{q}}{\mathrm{d}\,t} &= \frac{\mathrm{d}\,T}{\mathrm{d}\,\boldsymbol{p}} \\ \frac{\mathrm{d}\,\boldsymbol{p}}{\mathrm{d}\,t} &= -\frac{\mathrm{d}\,V}{\mathrm{d}\,\boldsymbol{q}} \end{cases}.$$

For a single body j, this gives us

$$\begin{cases} \frac{\mathrm{d}\,\boldsymbol{Q}_j}{\mathrm{d}\,t} &= \frac{\mathrm{d}\,T}{\mathrm{d}\,\boldsymbol{P}_j} = \frac{\mathrm{d}}{\mathrm{d}\,\boldsymbol{P}_j} \frac{1}{2} m_j v_j^2 = v \\ \frac{\mathrm{d}\,\boldsymbol{P}_j}{\mathrm{d}\,t} &= -\frac{\mathrm{d}\,V}{\mathrm{d}\,\boldsymbol{q}} \end{cases}.$$

In other words, the change in position is the velocity, and the change in momentum (the force) is in the direction which decreases the potential. It helps to visualise the potential for a two-dimensional problem, where the position of a body is given by x and y. One can plot the potential $V(x, y)$ as a hilly landscape, and the force is then directed downhill, its magnitude proportional to the slope of the hill. A one-dimensional example can be seen at `https://xkcd.com/681_large/`.

Let us for a moment consider a single body in a constant potential. Since the total energy is conserved, When the kinetic energy is 0, the body reaches its maximum height in the potential: it cannot be found at any point with a greater potential unless external energy is imparted to it. moreover, it cannot cross regions of higher potential.

It is therefore confined to some “lake” in the potential, whose height is defined by its energy.

TODO PICTURE