Introduction to symplectic integrator methods for solving diverse dynamical equations

Siu A. Chin

Department of Physics and Astronomy

Texas A&M University

College Station, TX, 77840, USA

Second Lecture

An example of the four formulations of classical mechanics, canonical transformations and Lie transforms.

Recall that in Lecture I we have briefly mentioned,

The **Four** formulations of mechanics:

1. **The Newtonian formulation:** Primarily just a second order differential equation as we have been using:

$$m\frac{d^2\mathbf{r}}{dt^2} = \mathbf{F}(\mathbf{r}).$$

For comparison with other formulations, we should express this in terms of the *momentum*

$$\mathbf{p} = m\frac{d\mathbf{r}}{dt}, \tag{5}$$

and the potential energy function $U(\mathbf{r})$

$$\mathbf{F}(\mathbf{r}) = -\nabla U(\mathbf{r}),$$

as a pair of equation (5) and below

$$\frac{d\mathbf{p}}{dt} = -\nabla U(\mathbf{r}). \tag{6}$$

2. **The Lagrangian formulation:** Generalize from Cartesian coordinates $r_i = (x, y, z)$, to *generalized coordinates* q_i such as *angles*, to satisfy constraints cumbersome to do so in terms of x, y, z. Corresponding to q_i are *generalize momentum*

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

where $\dot{q}_i = dq/dt$ and where the *Lagrangian function* is given by

$$L = \frac{1}{2} m \sum_i \dot{q}_i^2 - U(q_i).$$

The equation of motion is given by

$$\frac{\partial p_i}{\partial t} = \frac{\partial L}{\partial q_i}.$$

3. **The Hamiltonian formulation:** The most important key point. The generalized momenta p_i are to be regarded as *independent* fundamental dynamical degrees of freedom in equal footing as q_i. That is, p_i are NOT to be regarded as depending on $\dot{q}_i$, but rather, $\dot{q}_i$ are to be regarded as depending on p_i.

   The generalize momenta p_i are defined via L as before, but after that we eliminate all $\dot{q}_i$ by p_i in defining the Hamiltonian function

$$H(p_i, q_i) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i) = \frac{1}{2m} \sum_i p_i^2 + U(q_i).$$

   The dynamics is then given by the pair Hamilton's eqaution of motion:

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \quad \text{and} \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}.$$

4. **The Poissonian formulation:** Dynamics is expressed via *Poisson brackets*, which are canonically invariant. For any dynamical variable $W(q_i, p_i)$,

$$\begin{aligned}\frac{\partial W}{\partial t} &= \sum_i \Big(\frac{\partial W}{\partial q_i}\frac{\partial q_i}{\partial t} + \frac{\partial W}{\partial p_i}\frac{\partial p_i}{\partial t}\Big) \\ &= \sum_i \Big(\frac{\partial W}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial W}{\partial p_i}\frac{\partial H}{\partial q_i}\Big) \equiv \{W, H\} \\ &= \sum_i \Big(\frac{\partial H}{\partial p_i}\frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial}{\partial p_i}\Big) W\end{aligned}$$

which is of the form $\frac{\partial w}{\partial t} \equiv (T+V)w$ with operator solution:

$$W(t) = \mathrm{e}^{t(T+V)} W(0).$$

Since q_i and p_i are independent, we have the following *fundamental Poisson brackets*:

$$\{q_i, q_j\} = 0, \qquad \{p_i, p_j\} = 0, \qquad \{q_i, p_j\} = \delta_{ij}.$$

An illustrative example

Consider the case of a pendulum, consisted of a point mass m free to swing in the $x-y$ plane, of fixed length $r = \ell$, under the force of surface gravity with force $\mathbf{F} = (0, -mg)$:

The position of the mass point is

$$\mathbf{r} = (x, y) = r(\sin\theta, -\cos\theta) = r\hat{\mathbf{r}}$$

The motion must be constrainted to move such that $r = \ell$. The only degree of freedom is the swing angle θ.

In the Newtonian formulation, we must transform the acceleration vector to polar coordinates as follow:

$$\dot{\mathbf{r}} = \dot{r}\hat{\mathbf{r}} + r\dot{\hat{\mathbf{r}}} = \dot{r}\hat{\mathbf{r}} + r(\cos\theta, \sin\theta)\dot{\theta} = \dot{r}\hat{\mathbf{r}} + r\dot{\theta}\hat{\theta}$$

$$\begin{aligned}\ddot{\mathbf{r}} &= \ddot{r}\hat{\mathbf{r}} + \dot{r}\dot{\theta}\hat{\theta} + \dot{r}\dot{\theta}\hat{\theta} + r\ddot{\theta}\hat{\theta} + r\dot{\theta}(-\sin\theta, \cos\theta)\dot{\theta} \\ &= (\ddot{r} - r\dot{\theta}^2)\hat{\mathbf{r}} + (2\dot{r}\dot{\theta} + r\ddot{\theta})\hat{\theta}\end{aligned}$$

Therefore, Newton's second law in polar coordinate is given by

$$m(\ddot{r} - r\dot{\theta}^2) = F_r \quad \text{and} \quad m(2\dot{r}\dot{\theta} + r\ddot{\theta}) = F_\theta.$$

In order for the constraint $r = \ell$ to be satisfied, and hence $\dot{r} = 0$ and $\ddot{r} = 0$, we must have

$$F_r = -m\ell\dot{\theta}^2 \quad \text{and} \quad m\ell\ddot{\theta} = F_\theta$$

The first equation is the required radial force to enforce the constraint. If one simply assumes that the constaint is satisfied, then there is no need to even derive this equation in the first place. This is extra work in the Newtonian formulation.

From the geometry of the force diagram, it is easily seen that

$$F_\theta = -mg\sin\theta.$$

Hence, the equation in term of θ is just

$$m\ell\ddot{\theta} = -mg\sin\theta \quad \rightarrow \quad \ddot{\theta} = -\frac{g}{\ell}\sin\theta$$

Let's compare how the same problem is solved in the Lagrangian formulation. The Lagrangian function in 2D is

$$L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) - U(x, y)$$

Since $\mathbf{F} = (0, -mg)$, $U = mgy$. The constraint is expressed directly in terms of the generalize coordinate θ,

$$x = \ell \sin\theta, \quad y = -\ell\cos\theta, \qquad \dot{x} = \ell\cos\theta\dot{\theta}, \qquad \dot{y} = \ell\sin\theta\dot{\theta},$$

$$L = \frac{1}{2}m\ell^2\dot{\theta}^2 + mg\ell\cos\theta,$$

with generlized momentum

$$p_\theta = \frac{\partial L}{\partial\dot{\theta}} = m\ell^2\dot{\theta},$$

and equation of motion

$$\dot{p}_\theta = \frac{\partial L}{\partial\theta} \;\rightarrow\; m\ell^2\ddot{\theta} = -mg\ell\sin\theta \;\rightarrow\; \ddot{\theta} = -\frac{g}{\ell}\sin\theta.$$

There is no need to draw any diagram! (*Analytical Mechanics*)

In the Hamiltonian formulation, given the Lagrangian and the generlized momentum

$$L = \frac{1}{2}m\ell^2\dot{\theta}^2 + mg\ell\cos\theta, \qquad p_\theta = \frac{\partial L}{\partial\dot{\theta}} = m\ell^2\dot{\theta},$$

one forms the Hamiltonian by eliminating $\dot{\theta}$ in favor of p_θ,

$$H = p_\theta\dot{\theta} - L = p_\theta\dot{\theta} - \frac{1}{2}m\ell^2\dot{\theta}^2 - mg\ell\cos\theta$$

$$H = \frac{p_\theta^2}{2m\ell^2} - mg\ell\cos\theta,$$

giving Hamilton's equation

$$\dot{\theta} = \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{m\ell^2} \quad \dot{p}_\theta = -\frac{\partial H}{\partial\theta} = -mg\ell\sin\theta.$$

If the two equation *were* to be combined, then,

$$\rightarrow \quad m\ell^2\ddot{\theta} = -mg\ell\sin\theta \;\rightarrow\; \ddot{\theta} = -\frac{g}{\ell}\sin\theta.$$

In the Poissonian formulation,

$$\frac{\partial W}{\partial t} = \Big(\frac{\partial H}{\partial p_\theta}\frac{\partial}{\partial \theta} - \frac{\partial H}{\partial \theta}\frac{\partial}{\partial p_\theta}\Big)W.$$

If W were just θ or p_θ, then the Poisson equation-of-motion simply reproduce Hamilton's equation. However, the distinctive character of Poisson's equation is that it not only gives the equation satisfied by θ or p_θ, it gives their solution in an operator form:

$$W(t) = \mathrm{e}^{t\left(\frac{\partial H}{\partial p_\theta}\frac{\partial}{\partial \theta} - \frac{\partial H}{\partial \theta}\frac{\partial}{\partial p_\theta}\right)}W(0)$$

We will come back to this point later.

Canonical transformation

(How to derive algorithms with $\det M = 1$.)

For the standard Hamiltonian

$$H(q_i, p_i) = \sum_{i=1}^{n} \frac{p_i^2}{2m} + U(q_i), \qquad (1)$$

a canonical transformation $(q_i, p_i) \to (Q_i, P_i)$ is a transformation such that the new variables obey Hamilton's equations

$$\dot{Q}_i = \frac{\partial K}{\partial P_i}, \qquad \dot{P}_i = -\frac{\partial K}{\partial Q_i},$$

with respect to the transformed Hamiltonian $K(Q_i, P_i) = H(q_i, p_i)$.

Canonical transformations were first formulated in in terms of four types of *generating* functions, $F_1(q_k, Q_k, t)$, $F_2(q_k, P_k, t)$, $F_3(p_k, Q_k, t)$, $F_4(p_k, P_k, t)$. For our purpose, we will only need to use F_2 and F_3 without any explicit time-dependence, given by

$$p_i = \frac{\partial F_2(q_k, P_k)}{\partial q_i}, \qquad Q_i = \frac{\partial F_2(q_k, P_k)}{\partial P_i}, \tag{2}$$

and

$$q_i = -\frac{\partial F_3(p_k, Q_k)}{\partial p_i}, \qquad P_i = -\frac{\partial F_3(p_k, Q_k)}{\partial Q_i}. \tag{3}$$

If would take us too afar field to show and derived these transformation as canonical, but one can check that they have the very important property $\det M = 1$.

Consider the case of F_2 of Eq.(2). The first equation is an implicit equation for determining P_k in terms of q_i and p_i. The second, is an explicit equation for determining Q_i in terms of q_k *and* the updated P_k. This then can be naturally interpreted as a *sequence* of two transformations.

The first equation in (2) is the transformation $(q_i, p_i) \rightarrow (q_i^*, p_i^*)$ according to

$$p_i = \frac{\partial F_2(q_k, p_k^*)}{\partial q_i}, \qquad q_i^* = q_i,$$

with

$$\det M_1 = \det \frac{(\partial q_k^*, \partial p_k^*)}{(\partial q_i, \partial p_i)} = \det \frac{(\partial p_k^*)}{(\partial p_i)}.$$

The second equation is the transformation $(q_i^*, p_i^*) \rightarrow (Q_i, P_i)$ according to

$$P_i = p_i^*, \qquad Q_i = \frac{\partial F_2(q_i^*, P_i)}{\partial P_i},$$

with

$$\det M_2 = \det \frac{(\partial Q_k, \partial P_k)}{(\partial q_i^*, \partial p_i^*)} = \det \frac{(\partial Q_k)}{(\partial q_i^*)}.$$

The determinant of this two transformations is then

$$\det M = \det M_2 \det M_1 = \det \frac{(\partial Q_k)}{(\partial q_i^*)} \det \frac{(\partial p_k^*)}{(\partial p_i)}$$

$$= \det \frac{(\partial Q_k)}{(\partial q_i)} \Big/ \det \frac{(\partial p_i)}{(\partial P_k)} = 1.$$

The last equality follows from (2), since

$$\frac{\partial Q_k}{\partial q_i} = \frac{\partial F_2}{\partial q_i \partial P_k} = \frac{\partial p_i}{\partial P_k}.$$

Similarly for F_3. Thus a canonical transformation has $\det M = 1$, guarranteeing its stability.

The simplest canonical transformation is the identity transformation, for example given by

$$F_2 = \sum_{i=1}^{n} q_i P_i, \quad \rightarrow \quad p_i = \frac{\partial F_2}{\partial q_i} = P_i, \quad Q_i = \frac{\partial F_2}{\partial P_i} = q_i,$$

$$F_3 = -\sum_{i=1}^{n} p_i Q_i, \quad \rightarrow \quad q_i = -\frac{\partial F_3}{\partial p_i} = Q_i, \quad P_i = -\frac{\partial F_3}{\partial Q_i} = p_i.$$

The most important canonical transformation is when $Q_i = q_i(t)$ and $P_i = p_i(t)$, which describes the *dynamics* of the system at any t. Clearly, in this case, $K(Q_i, P_i) = H(q_i, p_i)$ and both the new and old variables obeys their respective Hamilton's equations. For an arbitrary t, the explicit transformation is generally unknown. However, when t is infinitesimally small, $t \to \Delta t$, it is well known that the Hamiltonian is the *infinitesimal* generator of time evolution. What was not realized for a long time is that even when Δt is *not* infinitesimally small, the resulting canonical transformation generated by the Hamiltonian, through no longer exact in evolving the system forward in time, remained an excellent numerical algorithm. Let's take

$$F_2(q_i, P_i) = \sum_{i=1}^{n} q_i P_i + \Delta t H(q_i, P_i) = \sum_{i=1}^{n} q_i P_i + \Delta t \Big[\sum_{i=1}^{n} \frac{P_i^2}{2m} + U(q_i) \Big].$$

For this generating function, Δt is simply an arbitrary parameter, need not be small. The transformation equations (2) then give,

$$P_i = p_i - \Delta t \frac{\partial U(q_i)}{\partial q_i}, \qquad Q_i = q_i + \Delta t \frac{P_i}{m} \tag{4}$$

If one regards $Q_i = q_i(\Delta t)$ and $P_i = p_i(\Delta t)$, then the above is precisely Cromer's algorithm. The transformation (4) is canonical regardless of the size of Δt, but it is an accurate scheme for evolving the system forward in time only when Δt is small. Similarly, taking

$$F_3(p_i, Q_i) = -\sum_{i=1}^{n} p_i Q_i + \Delta t H(Q_i, p_i) = -\sum_{i=1}^{n} p_i Q_i + \Delta t \Big[\sum_{i=1}^{n} \frac{p_i^2}{2m} + U(Q_i)\Big]$$

gives the other canonical algorithm

$$Q_i = q_i + \Delta t \frac{p_i}{m}, \qquad P_i = p_i - \Delta t \frac{\partial U(Q_i)}{\partial Q_i}.$$

Poisson mechanics and Lie transforms

The generating function method of constructing canonical is cumbersome in deriving more accurate, higher-order algorithm for solving classical dynamics problems. For a more efficient method, we need the Poissonian formulation of mechanics.

First, we review the operator form of Taylor's expansion

$$
\begin{aligned}
f(x+a) &= f(x) + a\frac{df}{dx} + \frac{1}{2}a^2\frac{d^2f}{dx^2} + \frac{1}{3!}a^3\frac{d^3f}{dx^3} + \cdots \\
&= (1 + a\frac{d}{dx} + \frac{1}{2}a^2\frac{d^2}{dx^2} + \frac{1}{3!}a^3\frac{d^3}{dx^3} + \cdots)f(x) \\
&= \mathrm{e}^{a\frac{d}{dx}}f(x).
\end{aligned}
$$

Thus the exponential of a first-order differential operator is a shift operator.

Recall Poisson's equation of motion,

$$W(t) = \mathrm{e}^{t(T+V)} W(0) = \mathrm{e}^{tH} W(0),$$

where

$$T = \sum_i \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} \qquad V = \sum_i -\frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} \qquad H = T + V.$$

For the most common, separable Hamiltonian

$$H(q_i, p_i) = \sum_{i=1}^{n} \frac{p_i^2}{2m} + U(q_i),$$

$$T = \sum_i \frac{p_i}{m} \frac{\partial}{\partial q_i} \qquad V = \sum_i F_i \frac{\partial}{\partial p_i}.$$

Let's define

$$\mathbf{v} \equiv \frac{\mathbf{p}}{m} \qquad \mathbf{a}(\mathbf{q}) = \frac{\mathbf{F}(\mathbf{q})}{m}$$

so that one can write

$$T = \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{q}} \qquad V = \mathbf{a}(\mathbf{q}) \cdot \frac{\partial}{\partial \mathbf{v}}.$$

Let's see how Poisson's operator solution solves the case of constant acceleration $\mathbf{a} = const$. The solution, we know, is

$$\frac{d^2\mathbf{q}}{dt^2} = \mathbf{a} \quad \rightarrow \quad \mathbf{q}(t) = \mathbf{q} + \mathbf{v}t + \frac{1}{2}\mathbf{a}t^2$$

where $\mathbf{q}$ and $\mathbf{v}$ are the initial values at $t = 0$. Poisson's solution is

$$\mathbf{q}(t) = \mathrm{e}^{tH} q = (1 + tH + \frac{1}{2}t^2H^2 + \frac{1}{3!}t^3H^3 \cdots)\mathbf{q}$$

$$H\mathbf{q} = \mathbf{v} \quad H^2\mathbf{q} = H\mathbf{v} = \mathbf{a} \quad H^3\mathbf{q} = H\mathbf{a} = 0, \quad H^4\mathbf{q} = 0, \quad \text{etc.}$$

Therefore, Poisson's solution is

$$\mathbf{q}(t) = \mathbf{q} + t\mathbf{v} + \frac{1}{2}t^2\mathbf{a}.$$

What happens now when $\mathbf{a}(\mathbf{q})$ is no longer constant? We now observe that

$$e^{tT}\binom{\mathbf{q}}{\mathbf{v}} = \binom{\mathbf{q}+t\mathbf{v}}{\mathbf{v}} \qquad e^{tV}\binom{\mathbf{q}}{\mathbf{v}} = \binom{\mathbf{q}}{\mathbf{v}+t\mathbf{a}(\mathbf{q})}.$$

That is, although $\exp(tT+tV)$ cannot be solved exactly, the component operator $\exp(tT)$ and $\exp(tV)$ are just shift operators, and can be evaluated exactly. This, therefore suggests that we should try to approximate

$$e^{t(T+V)} = \prod_i e^{a_i tT} e^{b_i tV}$$

to take advantage of the solvability of $\exp(tT)$ and $\exp(tV)$.

The advantage of this product decomposition or splitting is that the resulting algorithm is always a canonical transformation with $\det M = 1$!