§1 Introduction to Hamiltonian Systems

The theoretical, numerical, and computational areas of the field of particle methods are all based on the Hamiltonian formalism. We will introduce this formalism in this chapter and consider some of the mathematical properties, and the implications for the application.

1.1 Some Definitions and Notations

We consider a classical N particle system in $\mathbb{R}^3$.

"classical" $\hat{=}$ obey Newtonian mechanics

$$(1) \qquad \boxed{\underline{F}_i = m_i \ddot{q}_i} \qquad \begin{array}{l}\text{Newton's 2nd law} \\ i = 1, \dots, N\end{array}$$

$\underline{F}_i \in \mathbb{R}^3$: force experienced by particle i

$m_i \in \mathbb{R}$: mass of particle i

$q_i \in \mathbb{R}^3$: position of " "

$\dot{q}_i \in \mathbb{R}^3$: velocity of " "

$\ddot{q}_i \in \mathbb{R}^3$: acceleration " " "

Such a system can be defined as a collection of N points with position

$$q \in \mathbb{R}^{3N} \qquad \text{where} \quad q = (q_1, \dots, q_N)$$

and velocities

$$\dot{q} = \frac{d}{dt} q = \underline{v} \qquad \dot{q} \in \mathbb{R}^{3N}$$

The state of any particle system is completely defined by $(q, \dot{q})$. It is a deterministic system via (1) and 6N initial conditions $(q_0, \dot{q}_0)$.

1.2 Conservative Forces

We will restrict to conservative forces. Such vector fields ($\underline{F}$) are given as gradient fields of scalar potentials

$$\underline{F} = -\nabla_q V(q)$$

that in general depends on all coordinates of other particles.

Newton's 2nd law (1) is just an ODE (system)

$$\boxed{m_i \ddot{q}_i = -\nabla_{q_i} V(q)}$$

1.3 The Hamiltonian Formalism

One of the important properties of a Hamiltonian system is energy conservation.

How is energy defined?

$$E(q, \dot{q}) = V + K$$
$$= \underbrace{V(q)}_{\text{potential energy}} + \underbrace{\sum_{i=1}^{N} \frac{1}{2} m_i \dot{q}^2}_{\text{kinetic energy}}$$

Conservation implies that

$$\frac{d}{dt} E(q(t), \dot{q}(t)) = \sum_{i}^{N} \partial_{q_i} V(q)\, \dot{q}_i + \sum_{i=1}^{N} m_i \dot{q}_i \ddot{q}_i \overset{!}{=} 0$$

To study Hamiltonian systems more specifically, we need to rewrite the equations slightly using momenta instead of velocities

$$\boxed{p_i = m_i \dot{q}_i}$$

So for the whole system, we find

$$\underline{\underline{M}}\, \ddot{q} = -\nabla V(q) \qquad \underline{\underline{M}} = \operatorname{diag}(m_i)$$

$$\underline{\underline{M}}\, \dot{q} = p$$

with the energy

$$\boxed{E = H(q,p) = \sum_{i=1}^{N} \frac{1}{2m_i} p_i^2 + V(q)}$$

Hamiltonian (function)

Take gradients wrt p_i and q_i

$$\partial_{p_i} H = \frac{p_i}{m_i} = \frac{m_i \dot{q}_i}{m_i} = \boxed{\dot{q}_i = \partial_{p_i} H(q,p)}$$

$$\partial_{q_i} H = \partial_{q_i} V(q) \underset{\uparrow\ \text{Newton}}{=} -m_i \ddot{q}_i = -(m_i \dot{q}_i)^{\cdot} = -\dot{p}_i$$

$$\boxed{\begin{aligned} \dot{q} &= \nabla_p H(q,p) \\ \dot{p} &= -\nabla_q H(q,p) \end{aligned}}$$

Hamiltonian equations

Or, if we combine all:

$$\frac{d}{dt}\begin{pmatrix} \underline{q} \\ \underline{p} \end{pmatrix} = \underline{\underline{J}} \nabla H(\underline{q}, \underline{p})$$

with $\underline{\underline{J}} = \begin{pmatrix} \underline{\underline{0}} & \underline{\underline{I}} \\ -\underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \Rightarrow \underline{\underline{J}} = -\underline{\underline{J}}^T = -\underline{\underline{J}}^{-1}$

1.4 ODE properties of Hamiltonian Equations

We can also define a vector $\underline{x}(t)$ formed by the $6N$ dynamical variables of the system

$$\underline{x}(t) = (q_1, \dots, q_N, p_1, \dots, p_N)$$

Given $\underline{x}_0 = (q_0, p_0) \in \mathbb{R}^{6N}$

the Hamiltonian equations are of the form

$$\dot{\underline{x}} = f(\underline{x}) \qquad (f \text{ smooth})$$

and there is a unique solution

$$\phi_t(q_0, p_0) \longmapsto (q(t), p(t)) \qquad \in \mathbb{R}^{6N} \quad \forall t \in \mathbb{R}$$

$\phi_t(q_0, p_0)$ is a solution map – or phase flow – that maps from a point at $t=0$ to any other point t.

a) $\forall t \quad \phi_t : \mathbb{R}^{6N} \to \mathbb{R}^{6N}$ is a bijection, and

$$\phi_t^{-1} = \phi_{-t}$$

b) Hamiltonian is preserved under ϕ_t

$$H \circ \phi_t = H$$

$$H\left(\phi_t(q_0, p_0)\right) = H(q_0, p_0)$$

... and more ...

1.5 Physical Interpretation

- Hamiltonian Equations define a generalized velocity field in the $6N$ dimensional space of all $\{q_i(t), p_i(t)\}$.

- This $6N$ dimensional space is the phase space of the system.

- Each state of the system is uniquely defined by a single point $\underline{x}_0$ in phase space. The evolution of the system is defined by the phase trajectory ($\sim$ phase flow) $\underline{x}(t)$.

- Two separate trajectories $\underline{x}(t)$ and $\underline{x}'(t)$ cannot intersect, unless $\underline{x}_0 = \underline{x}_0'$, i.e. when the two trajectories are identical.