Classical equations of motion

- Several formulations
  - Newtonian
  - Lagrangian
  - Hamiltonian
- Advantages of non-Newtonian formulations
  - More general, no need for “fictitious” forces
  - Better suited for multiparticle systems
  - Better handling of constraints
  - Can be derived from more basic postulates
- Assume conservative forces:
  \[ F = - \nabla U \] (gradient of a scalar potential energy)
Newtonian formulation

- Cartesian spatial coordinates \( r_i = (x_i, y_i, z_i) \) are primary variables
  - \( N \) 2nd-order ordinary differential equations: \( m_i \frac{d^2 r_i}{dt^2} \equiv m_i \ddot{r}_i = F_i \)
- Example: 2D motion in a central force field
  \[
  m\ddot{x} = F \cdot \hat{x} = -f(r) \hat{r} \cdot \hat{x} = -xf(r) \\
  m\ddot{y} = F \cdot \hat{y} = -f(r) \hat{r} \cdot \hat{y} = -yf(r)
  \]
- Transform to polar coordinates
  \[
  mr^2 \dot{\theta} = \ell \quad \text{Constant angular momentum} \\
  m\ddot{r} = -f(r) + \frac{\ell^2}{mr^3} \quad \text{“Fictitious” force}
  \]
Lagrangian formulation

- Independent of coordinate system
- Define the Lagrangian $L(q, \dot{q}) \equiv K(q, \dot{q}) - U(q)$ and action $S = \int_{t_1}^{t_2} L(q, \dot{q}) dt$
- Equations of motion arise from the principle of least action (PLA) $\delta S = 0$

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} = 0, \quad j = 1, \ldots, N \quad (N \text{ 2nd-order differential equations})$$

- Central-force example: $L = K - U = \frac{1}{2}(m\ddot{r}^2 + r^2\dot{\theta}^2) - U(r)$

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{r}} \right) = \frac{\partial L}{\partial r} \Rightarrow m\ddot{r} = mr\ddot{\theta} - f(r) \quad \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{\theta}} \right) = \frac{\partial L}{\partial \theta} \Rightarrow \frac{d}{dt}(mr^2\dot{\theta}) = 0$$

$$F_r = - \nabla_r U = - f(r)\hat{r}$$
Hamiltonian formulation

- Appropriate for application to statistical and quantum mechanics
- Newtonian and Lagrangian viewpoints take the \( q_i \) as the fundamental variables
  - \( N \)-variable configuration space
  - \( \dot{q}_i \) appears only as convenient shorthand for \( dq/dt \)
- Formulas are 2nd-order differential equations
- Hamiltonian formulation seeks to work with 1st-order differential equations
  - \( 2N \) variables: phase space density of the \( N \)-body system
  - Treat the coordinate and its time derivative as independent variables
Mathematically, Lagrangian treats $q$ and $\dot{q}$ as distinct

- Identify generalized momentum as $p_j = \frac{\partial L}{\partial \dot{q}_j}$

Example:

- Lagrangian $L = K - U = \frac{1}{2}m\dot{q}^2 - U(q)$ and momentum $p = \frac{\partial L}{\partial \dot{q}} = m\dot{q}$

- Lagrangian equations of motion: $\frac{dp_j}{dt} = \frac{\partial L}{\partial q_j}$

We would like a formulation in which $p$ is an independent variable

- $p_i$ is the derivative of the Lagrangian with respect to $\dot{q}_i$ and we’re looking to replace $\dot{q}_i$ with $p_i$
• Using a Legendre transform, we can define the Hamiltonian

\[
H(q_j, p_j) = - \left( L(q_j, \dot{q}_j) - \sum_i p_i \dot{q}_i \right)
\]

\[
= - K(q_j, \dot{q}_j) + U(q_j) + \sum_i \frac{\partial K}{\partial \dot{q}_i} \dot{q}_i
\]

\[
= - \frac{1}{2} \sum_i m_i \dot{q}_i^2 + U(q_j) + \frac{1}{2} \sum_i (2m_i \dot{q}_i) \dot{q}_i
\]

\[
= + \frac{1}{2} \sum_i m_i \dot{q}_i^2 + U(q_j)
\]

\[
= K + U
\]
Hamiltonian formulation

- Hamiltonian’s equations of motion
- Rewrite Lagrangian equations in terms of momentum

Differential change in $L$:

$$dL = \frac{\partial L}{\partial q} dq + \frac{\partial L}{\partial \dot{q}} d\dot{q}$$

$$= \dot{p}dq + pd\dot{q}$$

Legendre transform:

$$H = - (L - p\dot{q})$$

$$dH = - \dot{p}dq + \dot{q}dp$$

Hamilton’s equation of motion:

$$\dot{q} = + \frac{\partial H}{\partial p}$$

$$\dot{p} = - \frac{\partial H}{\partial q}$$

Conservation of energy:

$$\frac{dH}{dt} = - \dot{p} \frac{dq}{dt} + \dot{q} \frac{dp}{dt} = 0$$

Lagrange’s equation of motion:

$$\frac{dp}{dt} = \dot{p} = \frac{\partial L}{\partial q}$$

Definition of momentum:

$$p = \frac{\partial L}{\partial \dot{q}}$$
Hamiltonian formulation

- Particle motion in a central force field

\[ H = K + U \]
\[ = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + U(r) \]

Hamilton's equations

\[ \dot{q} = + \frac{\partial H}{\partial q} \]
\[ (1) \quad \frac{dr}{dt} = \frac{p_r}{m} \]
\[ (2) \quad \frac{d\theta}{dt} = \frac{p_\theta}{mr^2} \]
\[ (3) \quad \frac{dp_r}{dt} = \frac{p_\theta}{mr^3} - f(r) \]
\[ (4) \quad \frac{dp_\theta}{dt} = 0 \]

Lagrange's equations

\[ (1) \quad m\ddot{r} = mr\dot{\theta}^2 - f(r) \]
\[ (2) \quad \frac{d}{dt}(mr^2\dot{\theta}) = 0 \]

- Equations equivalent, but theoretical basis is better
Phase space

- Complete picture of phase space
  - Full specification of micro state of the system is given by the values of all positions and all momentum of all bodies
    \[ G = (p_j, r_j) \]
  - View all positions and momenta as independent coordinates
    - Connection between them comes through equations of motion

- Motion through phase space
  - Helpful to think of dynamics as “simple” movement through phase space
    - Facilitates connection to quantum mechanics
    - Basis for theoretical treatment of dynamics
Integration algorithms

• Equations of motion in cartesian coordinates
\[
\frac{dr_j}{dt} = \frac{p_j}{m}
\]
\[
\frac{dp_j}{dt} = F_j = \sum_{i=1, i\neq j}^{N} F_{ij}
\]
(pairwise additive forces)

• Desirable features of an integrator
  • Minimal need to compute forces (expensive)
  • Good ability for large time steps
  • Good accuracy
  • Conserves energy and momentum
  • Time-reversible
  • Phase space area-preserving (symplectic)

More on these later
Time integration methods

• Let’s integrate a first-order ordinary differential equation (ODE):

\[ \frac{dS}{dt} = \dot{S}(t) = F(t, S(t)) \]

• Example: exponential function

\[ \dot{y} = e^{-t} \]

• A numerical approximation to the ODE is a set of values: \( \{ S_0, S_1, S_2, \ldots \} \) and \( \{ t_0, t_1, t_2, \ldots \} \)

• There are many different ways of obtaining this
Euler method

- Explicit Euler method: \( S_{n+1} = S_n + F(t_n, y_n) \Delta t \)
  - Simplest of all
  - Right-hand side depends on things already known: **explicit** method
  - The error in a single step is \( \mathcal{O}(\Delta t^2) \), but for \( N \) steps needed for a finite time interval, the total error scales as \( \mathcal{O}(\Delta t) \)!
  - Only first-order accurate, not advised to use!

- Implicit Euler method: \( S_{n+1} = S_n + F(t_{n+1}, y_{n+1}) \Delta t \)
  - Excellent stability properties
  - Suitable for stiff ODE
  - Requires implicit solver for \( y_{n+1} \) (i.e. more computations)
Predictor-corrector methods

- Predictor-corrector methods of solving initial value problems improve the approximation accuracy by querying the function several times at different locations (predictions), and then using a weighted average of the results (corrections) to update the state.

- Two formulas: the predictor and corrector
  - The **predictor** is an explicit formula and first estimates the solution at $t$, i.e. we can use Euler method or some other methods to finish this step.
  - Using the found $S(t_{n+1})$, the **corrector** can calculate a new, more accurate solution.
Midpoint

- Implicit midpoint method:
  \[ S_{n+1} = S_n + F \left( \frac{t_n + t_{n+1}}{2}, \frac{S_n + S_{n+1}}{2} \right) \Delta t \]
  
  - 2nd-order accurate
  - Time symmetric and symplectic
  - But still implicit
- Explicit midpoint method
  
  \[ S_{n+1} = S_n + F \left( t_n + \Delta t/2, S_n + F(t_n, S_n) \Delta t/2 \right) \Delta t \]
Runge-Kutta Motivation

- Runge-Kutta (RK) methods are one of the most widely used methods for solving ODEs.
- Euler method uses the first two terms in Taylor series to approximate the numerical integration

\[ S(t_{n+1}) = S(t_n + \Delta t) = S(t_n) + \dot{S}(t_n)\Delta t \]

- We can improve the accuracy of the numerical integration if we keep more terms!

\[ S(t_{n+1}) = S(t_n + \Delta t) = S(t_n) + \dot{S}(t_n)\Delta t + \frac{1}{2!} \ddot{S}(t_n)\Delta t^2 + \cdots + \frac{1}{m!} \frac{d^mS}{dt^m}(t_n)\Delta t^m \]

- In order to get this more accurate solution, we need to derive expressions for the higher order derivatives.
Runge-Kutta

- Runge-Kutta methods:
  - Whole class of integration methods

2nd-order accurate $\mathcal{O}(\Delta t^2)$

\[
    k_1 = F(t_n, S_n)
\]

\[
    k_2 = F(t_n + \Delta t, S_n + k_1 \Delta t)
\]

\[
    S_{n+1} = S_n + \left( \frac{k_1 + k_2}{2} \right) \Delta t
\]

4th-order accurate $\mathcal{O}(\Delta t^4)$

\[
    k_1 = F(t_n, S_n)
\]

\[
    k_2 = F(t_n + \Delta t/2, S_n + k_1 \Delta t/2)
\]

\[
    k_3 = F(t_n + \Delta t/2, S_n + k_2 \Delta t/2)
\]

\[
    k_4 = F(t_n + \Delta t, S_n + k_3 \Delta t/2)
\]

\[
    S_{n+1} = S_n + \left( \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} \right) \Delta t
\]