PHYS 141/241

Lecture 02: Newtonian/Lagrangian/Hamiltonian Mechanics

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Classical equations of motion

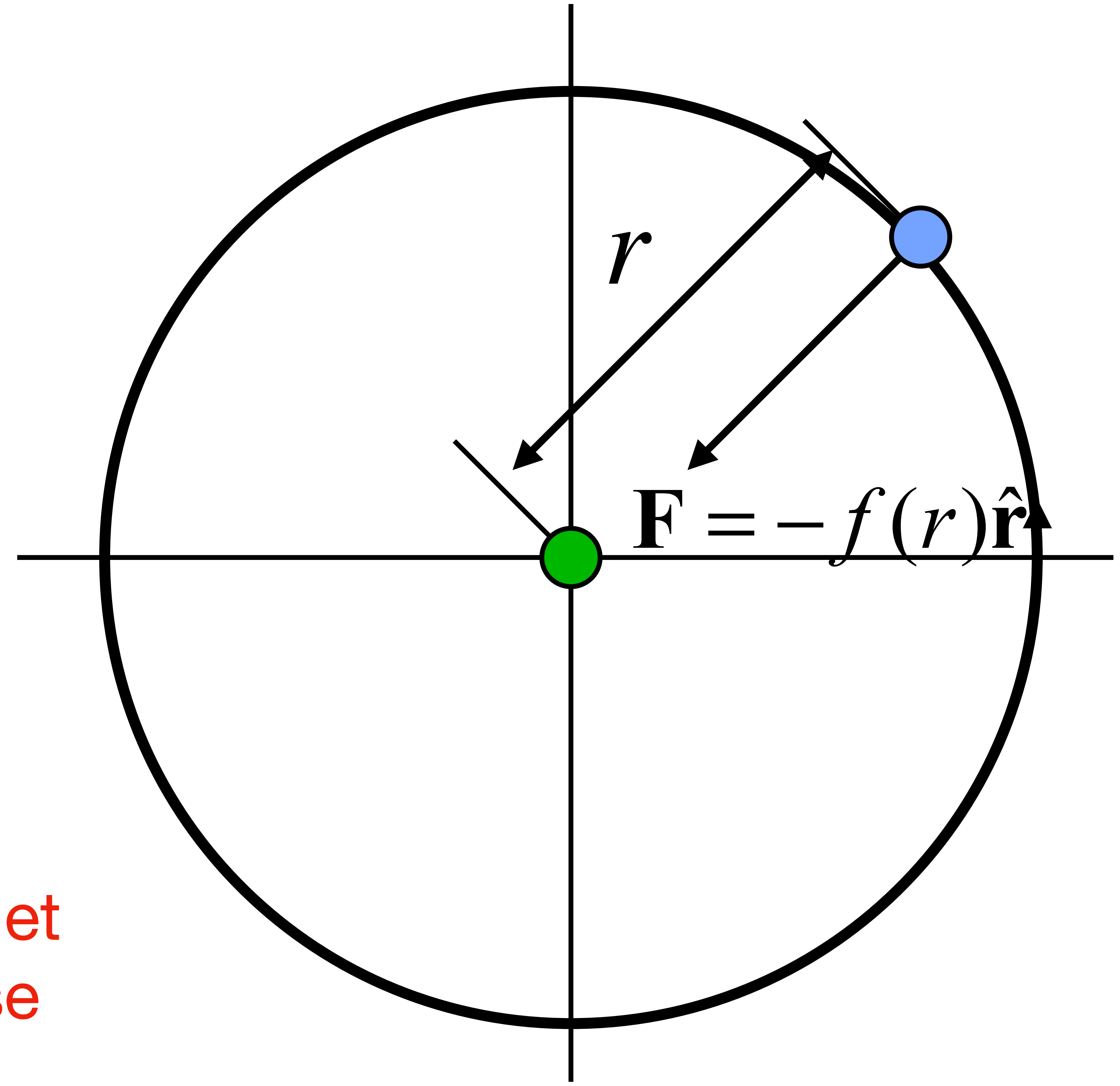
- Several formulations
  - Newtonian
  - Lagrangian
  - Hamiltonian
- Advantages of non-Newtonian formulations
  - More general, no need for “fictitious” forces
  - Better suited for multiparticle systems
  - Better handling of constraints
  - Can be derived from more basic postulates
- Assume conservative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

Newtonian formulation

- Cartesian spatial coordinates $\boldsymbol{r}_i = (x_i, y_i, z_i)$ are primary variables
  - N 2nd-order ordinary differential equations: $m_i \dfrac{d^2\boldsymbol{r}_i}{dt^2} \equiv m_i \ddot{\boldsymbol{r}}_i = \boldsymbol{F}_i$
- Example: 2D motion in a central force field

$$m\ddot{x} = \boldsymbol{F} \cdot \hat{x} = -f(r)\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{x}} = -xf(r)$$

$$m\ddot{y} = \boldsymbol{F} \cdot \hat{y} = -f(r)\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{y}} = -yf(r)$$



- Transform to polar coordinates

$$mr^2\dot{\theta} = \ell$$ Constant angular momentum

$$m\ddot{r} = -f(r) + \boxed{\frac{\ell^2}{mr^3}}$$ "Fictitious" force

Tedious to get general case

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) $\delta S = 0$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = 0, \qquad j = 1,\ldots,N$$

(N 2nd-order differential equations)

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

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

$\boldsymbol{F}_r = -\nabla_r U = -f(r)\hat{\boldsymbol{r}}$

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

Hamiltonian formulation

- Mathematically, Lagrangian treats q and $\dot{q}$ as distinct
  - Identify generalized momentum as $p_j = \dfrac{\partial L}{\partial \dot{q}_j}$
  - Example:
    - Lagrangian $L = K - U = \dfrac{1}{2}m\dot{q}^2 - U(q)$ and momentum $p = \dfrac{\partial L}{\partial \dot{q}} = m\dot{q}$
    - Lagrangian equations of motion: $\dfrac{\partial p_j}{dt} = \dfrac{\partial L}{\partial q_j}$
- 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

Hamiltonian formulation

- Using a *Legendre tranform*, we can define the Hamiltonian

$$
\begin{aligned}
H(q_j, p_j) &= -\left(L(q_j, \dot{q}_j) - \sum_i p_i \dot{q}_i \right) \\
&= -K(q_j, \dot{q}_j) + U(q_j) + \sum_i \frac{\partial K}{\partial \dot{q}_i} \dot{q}_i \\
&= -\frac{1}{2} \sum_i m_i \dot{q}_i^2 + U(q_j) + \frac{1}{2} \sum_i (2 m_i \dot{q}_i) \dot{q}_i \\
&= +\frac{1}{2} \sum_i m_i \dot{q}_i^2 + U(q_j) \\
&= K + U
\end{aligned}
$$

Hamiltonian formulation

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

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

Lagrange's equation of motion

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

Definition of momentum

Differential change in L:

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

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

Legendre transform:

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

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

$$\begin{cases} \dot{q} = +\dfrac{\partial H}{\partial p} \\ \dot{p} = -\dfrac{\partial H}{\partial p} \end{cases}$$

Hamilton's equation of motion

Conservation of energy: $\dfrac{\partial H}{dt} = -\dot{p}\dfrac{dq}{dt} + \dot{q}\dfrac{dp}{dt} = 0$

Hamiltonian formulation

Lagrange's equations

$$(1)\ m\ddot{r} = mr\dot{\theta}^2 - f(r)$$

$$(2)\ \frac{d}{dt}(mr^2\dot{\theta}) = 0$$

- Particle motion in a central force field

$$H = K + U$$

$$= \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + U(r)$$

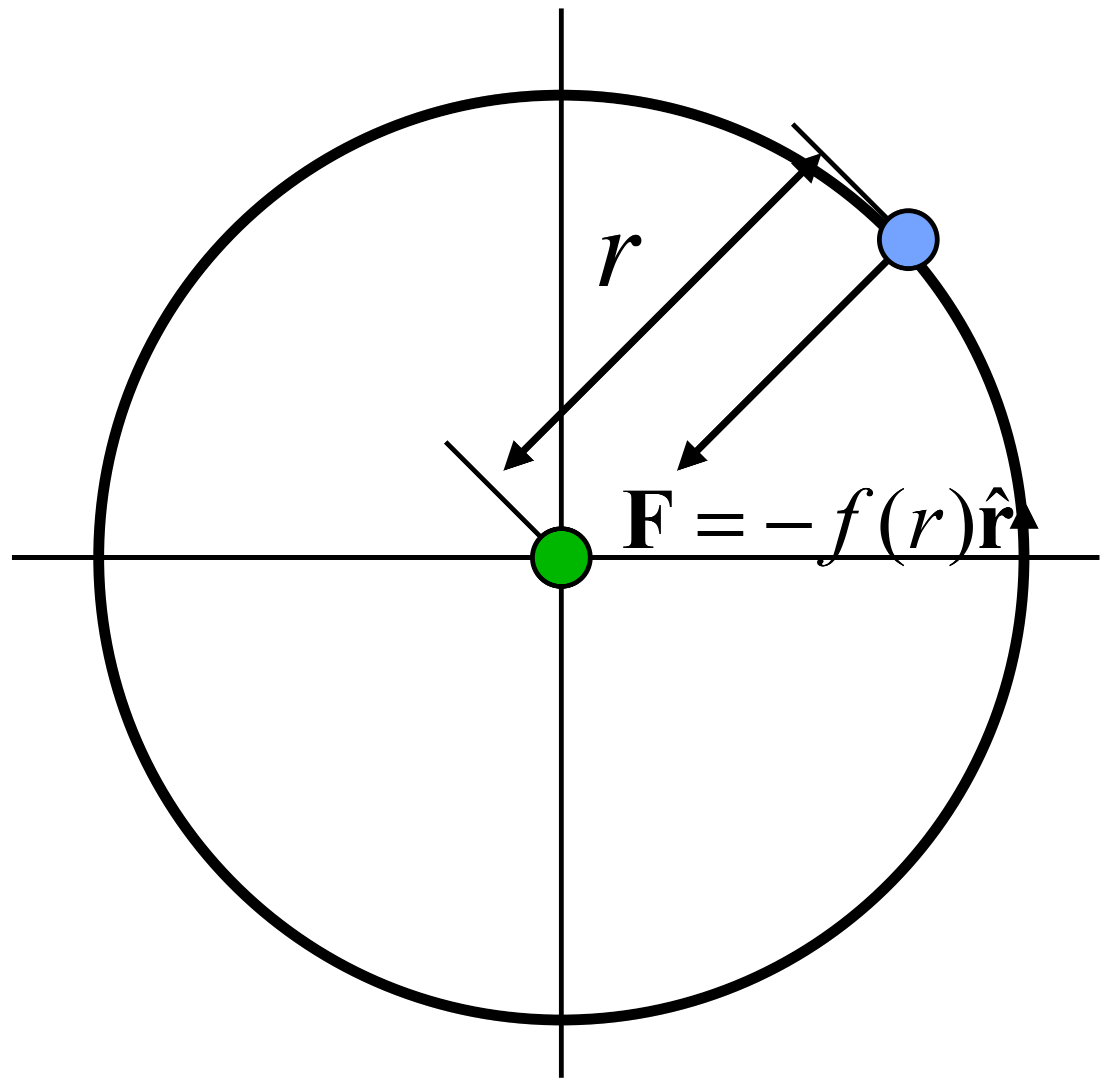
Hamilton's equations

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

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

$$(1)\ \frac{dr}{dt} = \frac{p_r}{m} \qquad (2)\ \frac{d\theta}{dt} = \frac{p_\theta}{mr^2}$$

$$(3)\ \frac{dp_r}{dt} = \frac{p_\theta}{mr^3} - f(r) \qquad (4)\ \frac{dp_\theta}{dt} = 0$$

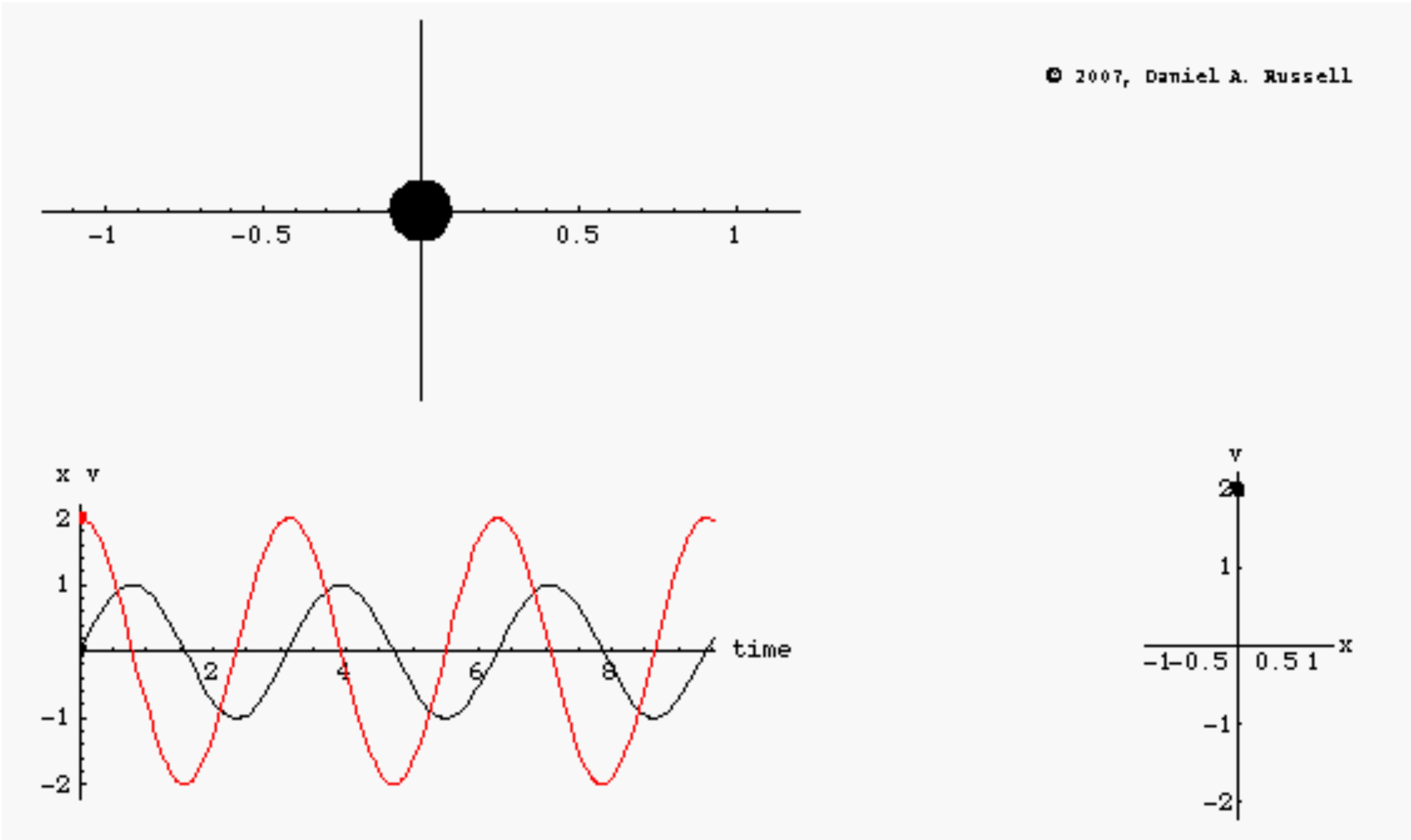


- Equations equivalent, but theoretical basis is better

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



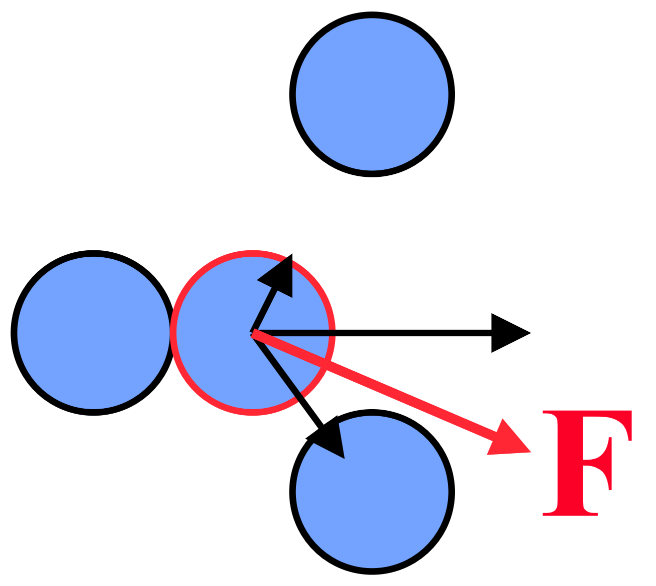
Integration algorithms

- Equations of motion in cartesian coordinates

$$\frac{d\boldsymbol{r}_j}{dt} = \frac{\boldsymbol{p}_j}{m}$$

$$\frac{d\boldsymbol{p}_j}{dt} = \boldsymbol{F}_j = \sum_{i=1,\, i\neq j}^{N} \boldsymbol{F}_{ij}$$

(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):

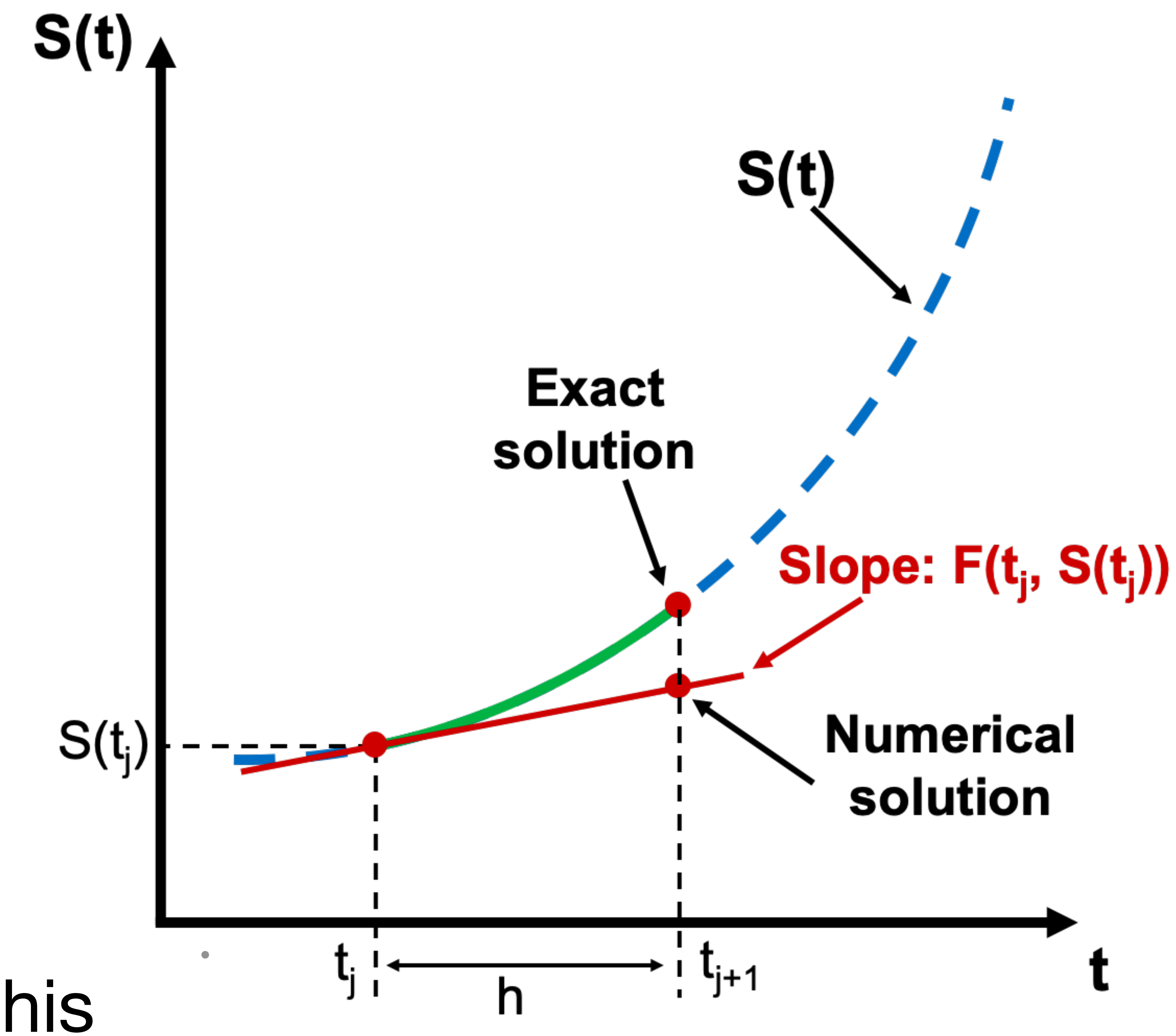
$$\frac{dS}{dt} = \dot{S}(t) = F(t, S(t))$$

- Example: exponential function

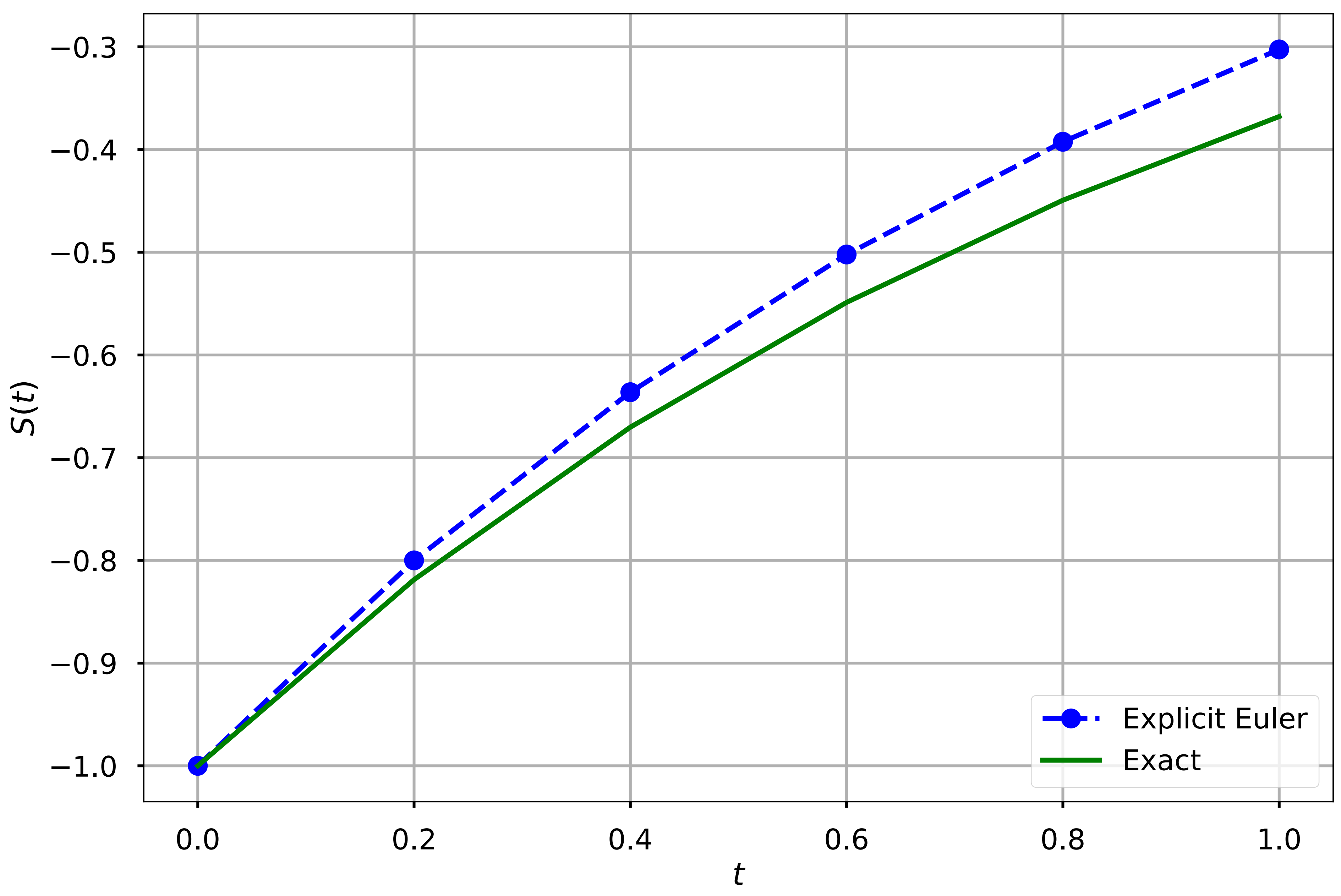
$$\dot{y} = e^{-t}$$

- 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

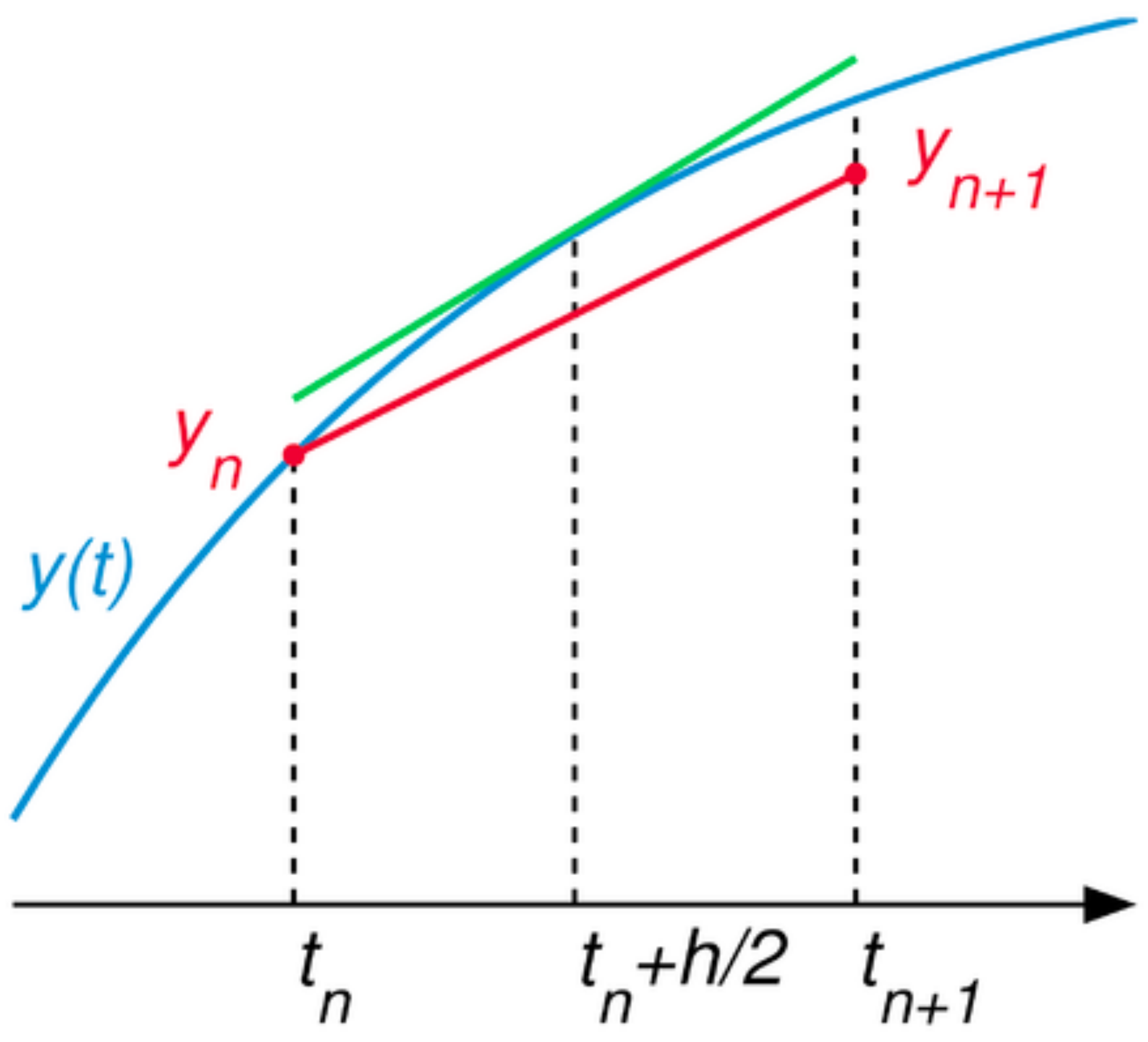
Midpoint

- 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!

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

- 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

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

$$k_1 = F(t_n, S_n)$$
$$k_2 = F(t_n + \Delta t/2, S_n + k_1 \Delta t/2)$$
$$k_3 = F(t_n + \Delta t/2, S_n + k_2 \Delta t/2)$$
$$k_3 = F(t_n + \Delta t, S_n + k_3 \Delta t/2)$$
$$S_{n+1} = S_n + \left(\frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6}\right)\Delta t$$

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

$$k_1 = F(t_n, S_n)$$
$$k_2 = F(t_n + \Delta t, S_n + k_1 \Delta t)$$
$$S_{n+1} = S_n + \left(\frac{k_1 + k_2}{2}\right)\Delta t$$