Lecture 2-3: Differential Equations (II)

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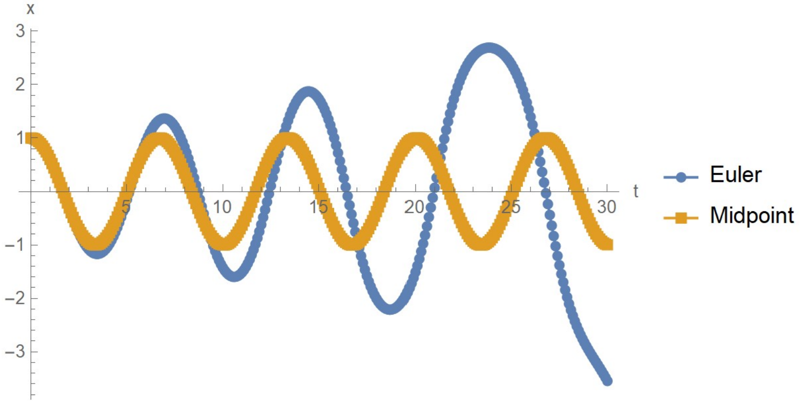
25. Oct. 2023

Last lecture

- Euler & midpoint methosd for 1st order ODEs.



Solution to $\dfrac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\sin(x)$ with (a large) $dt = 0.1$.

Today: Verlet method for integrating Newton's equations

Newton's equations for conservative system (where forces only depend on positions):

$$m_i \frac{\mathrm{d}^2 \boldsymbol{x}_i}{\mathrm{d}t^2} = -\boldsymbol{\nabla}_{\boldsymbol{x}_i} V(\{\boldsymbol{x}_j\}_j) \equiv \boldsymbol{F}_i(\{\boldsymbol{x}_j\}_j)\,,$$

for particles with masses m_i at positions $\boldsymbol{x}_i$ and interacting via the potential $V(\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N)$.
For example,

- Harmonic oscillator: $V(x) = \frac{1}{2}\omega^2 x^2$;
- Newtonian gravity: $V(\boldsymbol{x}_i) = -\frac{1}{2}\sum_{i\neq j} \frac{G m_i m_j}{|\boldsymbol{x}_i - \boldsymbol{x}_j|}$
- Molecular potential

Today: Verlet method for integrating Newton's equations

Generic form of the equation:

$$\frac{\mathrm{d}^2 \boldsymbol{x}(t)}{\mathrm{d}t^2} = \boldsymbol{a}[\boldsymbol{x}(t)] \,.$$

Idea of the algorithm:

- Evolve velocity for half a step:

$$\boldsymbol{v}\left(t + \frac{1}{2}\Delta t\right) \simeq \boldsymbol{v}(t) + \frac{1}{2}\boldsymbol{a}[\boldsymbol{x}(t)]\Delta t \,.$$

- Evolve position for a full step using the mid-point velocity:

$$\boldsymbol{x}(t + \Delta t) \simeq \boldsymbol{x}(t) + \boldsymbol{v}\left(t + \frac{1}{2}\Delta\right)\Delta t \,.$$

- Evolve velocity for another half step using acceleration at updated position:

$$\boldsymbol{v}(t + \Delta t) \simeq \boldsymbol{v}\left(t + \frac{1}{2}\Delta t\right) + \frac{1}{2}\boldsymbol{a}[\boldsymbol{x}(t + \Delta t)]\Delta t \,.$$

In case you wonder why ...

Suppose (for a single particle in 1D) we want to find the dynamics of a function $\phi(t) \equiv \phi[x(t), p(t)]$ depending only on position x and momentum $p = mv$.
One get from Hamiltonian mechanics:

$$\phi(t) = \mathrm{e}^{\mathrm{i}\mathcal{L}t}\phi(0)\,, \quad \mathrm{i}\mathcal{L}(\bullet) = \frac{p}{m}\cdot\frac{\partial(\bullet)}{\partial x} + F\cdot\frac{\partial(\bullet)}{\partial p}\,.$$

- The generator has two non-commuting parts:

$$\mathrm{i}\mathcal{L} = \mathrm{i}\mathcal{L}_1 + \mathrm{i}\mathcal{L}_2\,, \quad \mathrm{i}\mathcal{L}_1(\bullet) \equiv \frac{p}{m}\cdot\frac{\partial(\bullet)}{\partial x}\,, \quad \mathrm{i}\mathcal{L}_2(\bullet) \equiv F\cdot\frac{\partial(\bullet)}{\partial p}\,, \quad [\mathrm{i}\mathcal{L}_1, \mathrm{i}\mathcal{L}_2] \neq 0\,.$$

- Trotter theorm (1959) implies:

$$\mathrm{e}^{\mathrm{i}\mathcal{L}\Delta t} = \mathrm{e}^{\mathrm{i}\mathcal{L}_2\Delta t/2}\cdot\mathrm{e}^{\mathrm{i}\mathcal{L}_1\Delta t}\cdot\mathrm{e}^{\mathrm{i}\mathcal{L}_2\Delta t/2} + \mathcal{O}(\Delta t^3)\,.$$

- Read more here — Trotter derived algorithms for molecular dynamics with constraints: Velocity Verlet revisited.

Verlet Method: summary

Algorithm: velocity-Verlet Method

Input: acceleration function $\boldsymbol{a}(\boldsymbol{x})$, initial values t_0, $\boldsymbol{x}_0$, $\boldsymbol{v}_0$ step size Δt, and final time t_f.

1. set $t = t_0$, $\boldsymbol{x} = \boldsymbol{x}_0$, $\boldsymbol{v} = \boldsymbol{v}_0$.
2. repeat $N = \lceil t_f / t_0 \rceil$ times:
   - set $\boldsymbol{v} = \boldsymbol{v} + \boldsymbol{a}(\boldsymbol{x})\Delta t/2$,
   - set $\boldsymbol{x} = \boldsymbol{x} + \boldsymbol{v}\Delta t$,
   - set $\boldsymbol{v} = \boldsymbol{v} + \boldsymbol{a}(\boldsymbol{x})\Delta t/2$.

Output: the sequence of t, $\boldsymbol{x}$ and $\boldsymbol{v}$ approximating the solution of $\frac{\mathrm{d}^2\boldsymbol{x}}{\mathrm{d}t^2} = \boldsymbol{a}(\boldsymbol{x})$.

Comparison with Euler method

Input: Same as left

1. Same as left
2. repeat N times:
   - set $\boldsymbol{a}_t = \boldsymbol{a}(\boldsymbol{x})$,
   - set $\boldsymbol{x} = \boldsymbol{x} + \boldsymbol{v}\Delta t$,
   - set $\boldsymbol{v} = \boldsymbol{v} + \boldsymbol{a}_t\Delta t$.

Output: the sequence of t, $\boldsymbol{x}$ and $\boldsymbol{v}$.

- Good numerical stability and other important physical properties: time reversibility and preservation of the symplectic form on phase space, at no significant additional computational cost over the simple Euler method.

Assignment 13

Write a `Fortran` program that solves the equation of motion for a frictionless physical pendulum (again) using the velocity-Verlet method: $\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\sin(x)$.

- You can base your program on the previous assignment (hint: see the comparison on the previous slide).
- Solve with the initial conditions `t0=0, x0=1.0, v0=0.0` and `dt = 0.1, tf=30`.
- The program should create a file (`verlet.txt`) with the result in three columns: `t`, `x(t)` and `v(t)`.
- Plot the result x versus t with your favorite plotting program.

Bonus question:

- Expand your subroutines and solve the equation of motion for a point mass in a gravitational field (moving in a 2D plane): $\frac{\mathrm{d}^2 \boldsymbol{x}}{\mathrm{d}t^2} = -\boldsymbol{x}/|\boldsymbol{x}|^3$ using the euler and verlet methods, with initial conditions `t0=0, x0=(/2.0, 0.0/), v0 = (/0.0, 0.5/)` and `dt = 0.1, tf=30`. Plot the trajectory [$x(1)$ vs $x(2)$] and compare the performance between the two methods.

Submit the graphs and your code as `Ass13.YourLastName.f90` to `li.zejian@ictp.it` before the next lesson.