Particle Trajectory Calculation in SPH

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Outline

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- Numerical method
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- Error analysis
- Summary

Background

The oil spill, sewage effluent, sediment flow and air haze

Governing equation

- Particle trajectory equation

$$\frac{d\overrightarrow{x_i}}{dt} = \overrightarrow{v_i}\left(t, \overrightarrow{x_i}\right)$$

$\overrightarrow{x_i}$: i particle coordinate

$\overrightarrow{v_i}$: local velocity (depend on the particle position)

Numerical method

Euler Method:

$$\vec{x}_i^{\,n+1} = \vec{x}_i^{\,n} + \Delta t \vec{v}_i \left(t^n, \vec{x}_i^{\,n} \right)$$

Modified Euler:

predictor step: $\vec{x}_i^{\,n+1,p} = \vec{x}_i^{\,n} + \Delta t \vec{v}_i^{\,n}$ where: $\vec{v}_i^{\,n} := \vec{v}_i \left(t^n, \vec{x}_i^{\,n} \right)$

corrector step: $\vec{x}_i^{\,n+1} = \vec{x}_i^{\,n} + \Delta t \dfrac{\vec{v}_i^{\,n} + \vec{v}_i^{\,n+1,p}}{2}$

Numerical method

Second-Order Runge-Kutta (RK2):

$$\vec{x}_i^{\,n+1} = \vec{x}_i^{\,n} + k_2$$

$$k_2 = \Delta t \vec{v}_i \left(t^n + \frac{\Delta t}{2}, \vec{x}_i^{\,n} + \frac{k_1}{2} \right)$$

$$k_1 = \Delta t \vec{v}_i \left(t^n, \vec{x}_i^{\,n} \right)$$

Fourth-Order Runge-Kutta (RK4):

$$\vec{x}_i^{\,n+1} = \vec{x}_i^{\,n} + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)$$

$$k_1 = \Delta t \vec{v}_i \left(t^n, \vec{x}_i^{\,n} \right)$$

$$k_2 = \Delta t \vec{v}_i \left(t^n + \frac{\Delta t}{2}, \vec{x}_i^{\,n} + \frac{k_1}{2} \right)$$

$$k_3 = \Delta t \vec{v}_i \left(t^n + \frac{\Delta t}{2}, \vec{x}_i^{\,n} + \frac{k_2}{2} \right)$$

$$k_4 = \Delta t \vec{v}_i \left(t^n + \Delta t, \vec{x}_i^{\,n} + k_3 \right)$$

Numerical method

***Velocity Verlet*:**

$$\vec{x}_i^{\,n+1} = \vec{x}_i^{\,n} + \vec{v}_i^{\,n}\Delta t + \frac{1}{2}\vec{a}_i^{\,n}\Delta t^2$$

$$\vec{v}_i^{\,n+1} = \vec{v}_i^{\,n} + \frac{1}{2}\Delta t\left(\vec{a}_i^{\,n+1} + \vec{a}_i^{\,n}\right)$$

***Leap Frog*:**

$$\vec{v}_i^{\,n+1/2} = \vec{v}_i^{\,n-1/2} + \vec{a}_i^{\,n}\Delta t$$

$$\vec{x}_i^{\,n+1} = \vec{x}_i^{\,n} + \vec{v}_i^{\,n+1/2}\Delta t$$

$$\vec{v}_i^{\,n} = \frac{1}{2}\left(\vec{v}_i^{\,n+1/2} + \vec{v}_i^{\,n-1/2}\right)$$

i particle acceleration: $\vec{a}_i = d\vec{x}_i / dt$

Experimental results

- Example

Flow field:

$$v_x = ax - by$$

$$v_y = ay + bx$$

x and y are the cartesian coordinates

Exact solution:

$$x(t) = \exp(at)\left[x_0 \cos bt - y_0 \sin bt\right]$$

$$y(t) = \exp(at)\left[x_0 \sin bt + y_0 \cos bt\right]$$

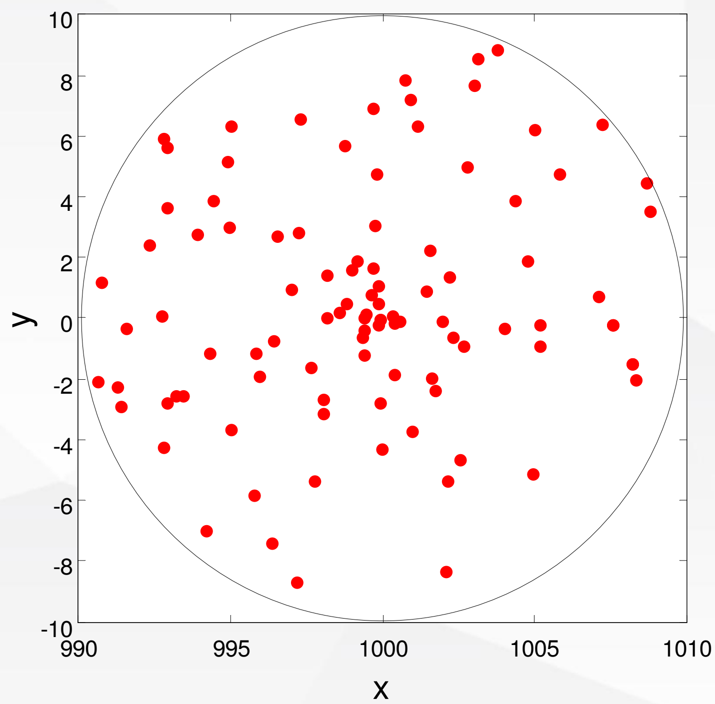
Initial particle coordinates: x_0=1000 y_0=0 $a = 0$

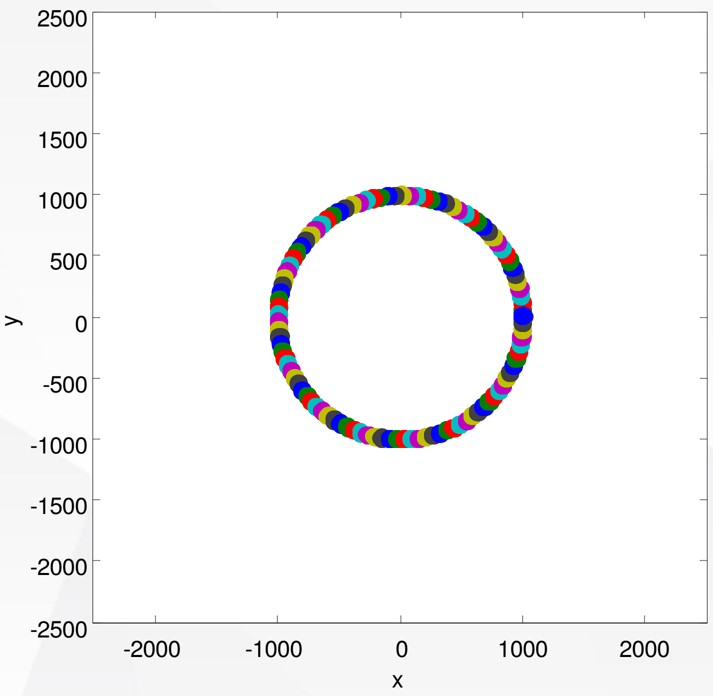
time interval 60 s total run time is 4000π h $b = 0.001$

Experimental results

N=100 particles variance
Measure dispersion
Particle cluster

The exact solution

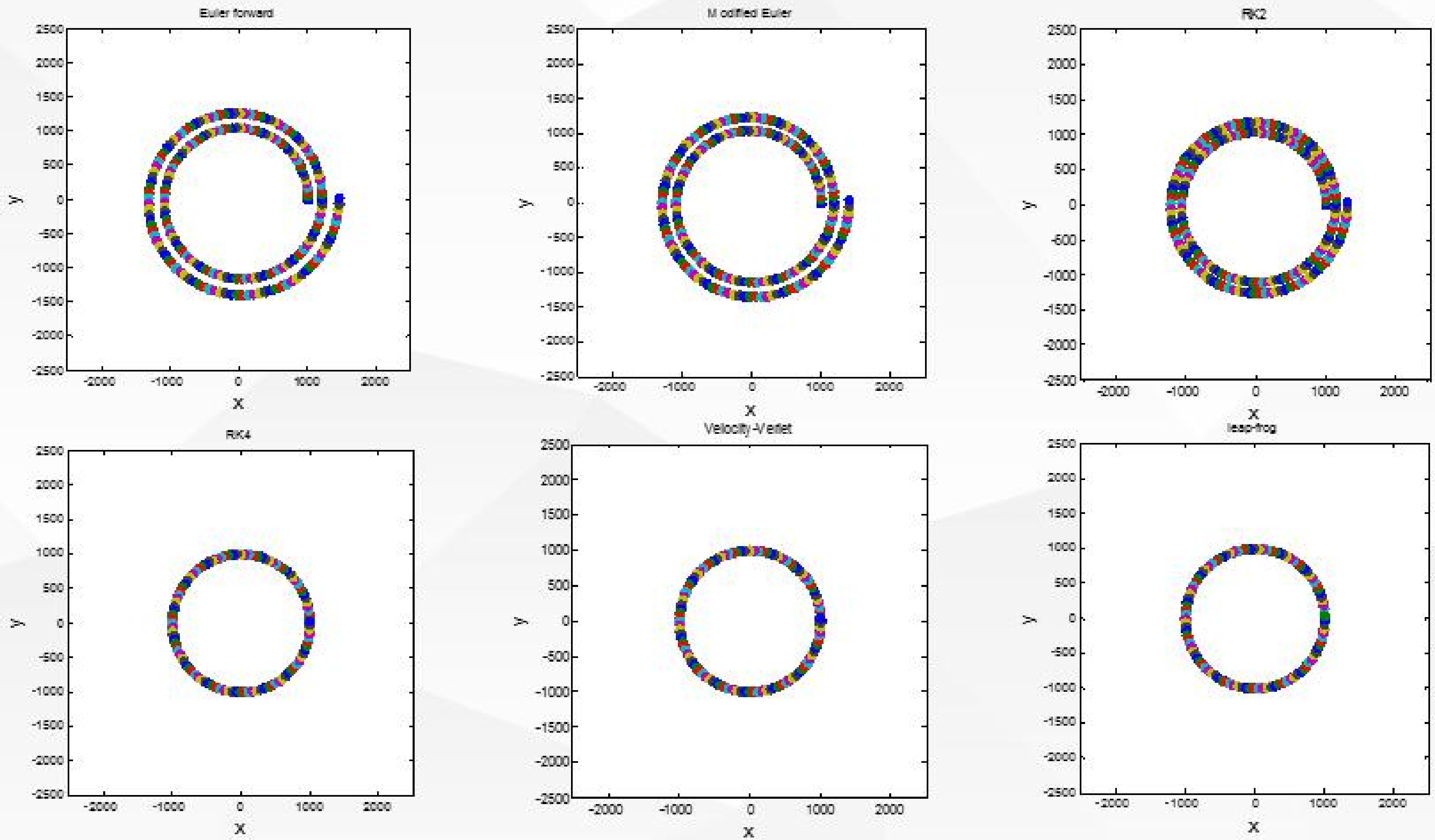




Experimental results

The six time stepping schemes for particle trajectory

ca



Error analysis

1. Theoretical error analysis:

Taylor series expansion:

$$f(t_{i+1}) = f(t_i) + \Delta t \cdot f'(t_i) + \frac{\Delta t^2}{2} f''(t_i) + \frac{\Delta t^3}{6} f'''(t_i) + \cdots$$

E.g. Euler forward time stepping, neglecting second and higher-order derivative terms:

$$f'(t_i) = \frac{f(t_{i+1}) - f(t_i)}{\Delta t}$$

In fact:

$$f'(t_i) = \frac{f(t_{i+1}) - f(t_i)}{\Delta t} - \frac{\Delta t}{2} f''(t_i) - \frac{\Delta t^2}{6} f'''(t_i) + \cdots$$

Truncation error:

$$TE = -\frac{\Delta t}{2} f''(t_i) - \frac{\Delta t^2}{6} f'''(t_i) + \cdots$$

Error analysis

2. Numerical error analysis:

$$\text{error} = \text{average}\sqrt{\sum_t \left(\frac{\left(x_{num}^t - x_{exact}^t\right)^2}{\left(x_{exact}^t\right)^2} + \frac{\left(y_{num}^t - y_{exact}^t\right)^2}{\left(y_{exact}^t\right)^2} \right)}$$

$\left(x_{num}^t, y_{num}^t\right)$: the coordinates obtained numerically at t time step

$\left(x_{exact}^t, y_{exact}^t\right)$: the exact coordinates at t time step

Error Analysis

2.1 Euler error values for different time steps

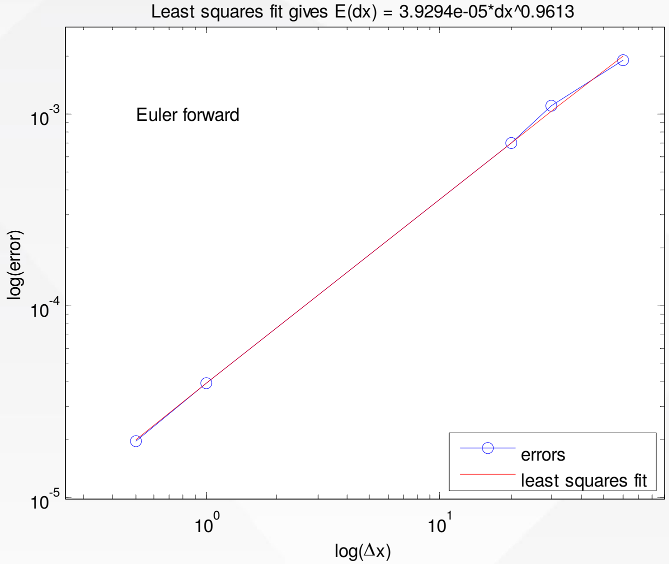
Δt (h) / Error	**0.5**	**1**	**20**	**30**	**60**
Euler	1.9866×10^{-5}	3.9563×10^{-5}	7.0257×10^{-4}	0.0011	0.0019

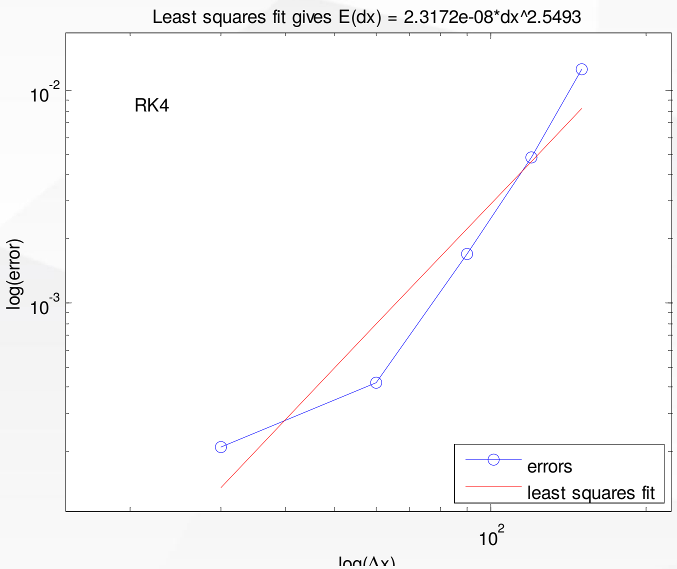
2.2 RK4 and Velocity Verlet error values for different time steps

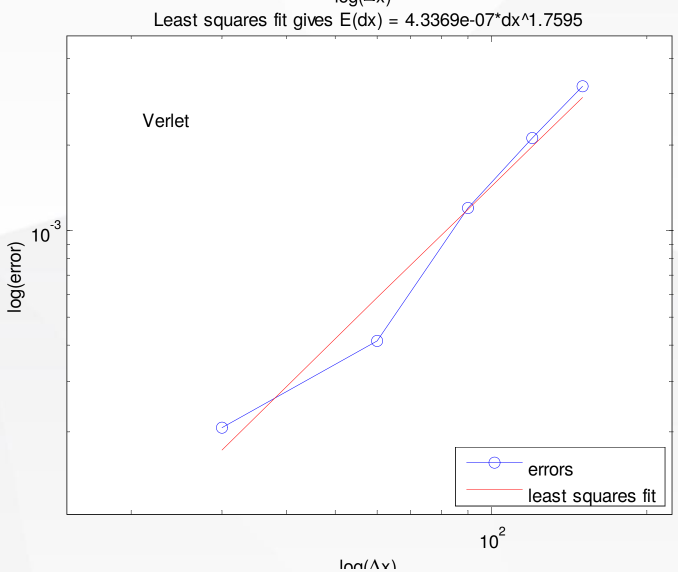
Δt (h) / Error	**30**	**60**	**90**	**120**	**150**
RK4	2.1003×10^{-4}	4.1892×10^{-4}	0.0017	0.0048	0.0125
Velocity Verlet	2.0728×10^{-4}	4.1338×10^{-4}	0.0012	0.0021	0.0032

Error analysis

Euler forward, RK4 and velocity Verlet error values in different time steps, and draw corresponding **convergence rate** curves







Summary

- Euler, modified Euler and RK2 may not predict accurate particle trajectories, introduce varying degrees of artificial dispersion
- RK4, velocity Verlet and leap frog can accurately calculate the particle trajectories without artificial dispersion
- Through error analysis and convergence rate experiments, we found that convergence rate can be different from accuracy for the same method

THANKS