

Time Integration



After discretization in space, partial differential equation reduces to a ordinal differential equation in time.

$$\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = 0$$



Ordinal diff. eq.

$$\frac{\partial f}{\partial t} = -u_j \frac{f_j - f_{j-1}}{\Delta x}$$

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Taylor-expansion series



$$f(t^{n+1}) = f(t^n + \Delta t)$$

$$= f(t^n) + \left. \frac{df}{dt} \right|_{t=t^n} \Delta t + \frac{1}{2} \left. \frac{d^2 f}{dt^2} \right|_{t=t^n} \Delta t^2 + \frac{1}{6} \left. \frac{d^3 f}{dt^3} \right|_{t=t^n} \Delta t^3 \dots$$

1st order approximation: $\frac{f^{n+1} - f^n}{\Delta t} = \left. \frac{\partial f}{\partial t} \right|^n$

Advection equation

$$\frac{\partial f}{\partial t} = -u \frac{\partial f}{\partial x} \quad \rightarrow \quad f^{n+1} = f^n - u \left. \frac{\partial f}{\partial x} \right|^n \Delta t$$

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Semi-Lagrangian Scheme(1/2)



Advection equation : relation between time and space

$$\frac{\partial f}{\partial t} = -u \frac{\partial f}{\partial x} \quad \frac{\partial^2 f}{\partial t^2} = u^2 \frac{\partial^2 f}{\partial x^2} \quad \frac{\partial^3 f}{\partial t^3} = -u^3 \frac{\partial^3 f}{\partial x^3}$$

Substituting into the Taylor-expansion series,

$$\begin{aligned} f^{n+1} &= f^n - u \left. \frac{\partial f}{\partial x} \right|^n \Delta t + \frac{1}{2} u^2 \left. \frac{\partial^2 f}{\partial x^2} \right|^n \Delta t^2 + \frac{1}{6} u^3 \left. \frac{\partial^3 f}{\partial x^3} \right|^n \Delta t^3 + \dots \\ &= f^n - \left. \frac{\partial f}{\partial x} \right|^n (u \Delta t) + \frac{1}{2} \left. \frac{\partial^2 f}{\partial x^2} \right|^n (u \Delta t)^2 + \frac{1}{6} \left. \frac{\partial^3 f}{\partial x^3} \right|^n (u \Delta t)^3 + \dots \end{aligned}$$

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Semi-Lagrangian Scheme(2/2)



Interpolation function in local region:

$$\begin{aligned} F(x) &= ax^3 + bx^2 + cx + f_j \\ \left. \frac{\partial^3 f}{\partial x^3} \right|_j &= 6a \quad \left. \frac{\partial^2 f}{\partial x^2} \right|_j = 2b \quad \left. \frac{\partial f}{\partial x} \right|_j = c \end{aligned}$$

Substituting into the Taylor-expansion series,

$$\begin{aligned} f^{n+1} &= f^n - c(u \Delta t) + b(u \Delta t)^2 - a(u \Delta t)^3 + \dots \\ &= F(-u \Delta t) \end{aligned}$$

CIP / Cubic Semi-Lagrangian operation

= 3rd-order time integration

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Predictor-Corrector



$f(t)$ is a dependent variable of t ,

Ordinal differential equation: $\frac{df}{dt} = S(y, t)$

Integrating from t^n to t^{n+1} ,

$$f^{n+1} = f^n + \int_{t^n}^{t^{n+1}} S(f, t) dt$$

The integration can not be done explicitly, because f is included in the non-analytical function S .

Definition : $f^n \equiv f(t^n)$, $S^n \equiv S(f^n, t^n)$

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Prediction Phase



By using the n -step (current step) f^n value and r -numbers previous time-step values, f^{n-1} , f^{n-2} , $\dots$ f^{n-r} ,

Approximate function of $S(f, t)$ can be constructed.

Using f^n and f^{n-1} , the 1st-order function :

$$S_p^1 = \frac{t - t^{n-1}}{\Delta t} S^n - \frac{t - t^n}{\Delta t} S^{n-1} + O(\Delta t)$$

By substituting into the integration, we have

$$\begin{aligned} f_p^{n+1} &= f^n + \int_{t^n}^{t^{n+1}} S_p^1(f, t) dt \\ &= f^n + \frac{\Delta t}{2} (3S^n - S^{n-1}) + O(\Delta t^2) \end{aligned}$$

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Higher-order Prediction



Using the more previous values, the more accurate predictions are obtained

$$r=2: \quad y_p^{n+1} = y^n + \frac{\Delta t}{12} (23f^n - 16f^{n-1} + 5f^{n-2}) + O(\Delta t^3)$$

$$r=3: \quad y_p^{n+1} = y^n + \frac{\Delta t}{24} (55f^n - 59f^{n-1} + 37f^{n-2} - 9f^{n-3}) + O(\Delta t^4)$$

$$r=4: \quad y_p^{n+1} = y^n + \frac{\Delta t}{720} (1901f^n - 2774f^{n-1} + 2616f^{n-2} - 1274f^{n-3} + 251f^{n-4}) + O(\Delta t^5)$$

These are called Adams – Bashforth formula.
(J.C.Adams – F.Bashforth)

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Correction Phase



Getting f_p^{n+1} enables us to construct $S^{n+1} = S(f_p^{n+1}, t^{n+1})$.

Using f_p^{n+1} , f^n , f^{n-1} , $\dots$ f^{n-r+1} ,

r -th-order polynomial function can be constructed.

1st-order approximate function:

$$S_c^1 = \frac{t - t^n}{\Delta t} S^{n+1} + \frac{t^{n+1} - t}{\Delta t} S^n + O(\Delta t)$$

By substituting into the integration, we have the corrected value.

$$\begin{aligned} f_c^{n+1} &= f^n + \int_{t^n}^{t^{n+1}} S_c^1(y, t) dt \\ &= f^n + \frac{\Delta t}{2} (S^{n+1} + S^n) \end{aligned}$$

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Higher-order Correction



$$r = 2: \quad y_c^{n+1} = y^n + \frac{\Delta t}{12} (5f^{n+1} + 8f^n - f^{n-1})$$

$$r = 3: \quad y_c^{n+1} = y^n + \frac{\Delta t}{24} (9f^{n+1} + 19f^n - 5f^{n-1} + f^{n-2})$$

$$r = 4: \quad y_c^{n+1} = y^n + \frac{\Delta t}{720} (251f^{n+1} + 646f^n - 264f^{n-1} + 106f^{n-2} - 19f^{n-3})$$

These are called the Adams–Moulton formula.
(J.C.Adams – F.R.Moulton)

Repetition of the prediction-correction loop improves the accuracy of the convergence.

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Runge-Kutta Method



$$\frac{df}{dt} = S(y, t)$$

1-stage RK Method (1st-Order Euler)

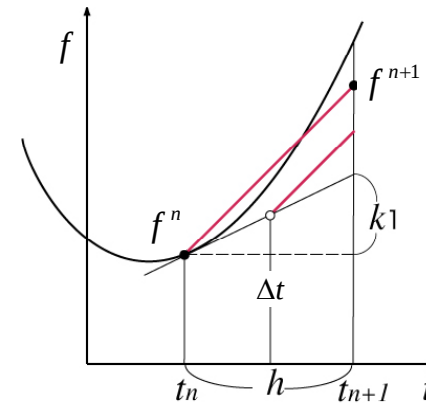
$$f^{n+1} = f^n + \Delta t S(f^n, t^n) + \underline{O(\Delta t^2)}$$

2-stage RK Method

$$k_1 = \Delta t S(x_n, t_n)$$

$$f^{n+1} = f^n + \Delta t S(f^n + 1/2k_1, t^n + 1/2\Delta t) + \underline{O(\Delta t^3)}$$

$O(\Delta t^2)$ error can be eliminated.



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4-Stage Runge-Kutta



By eliminating higher-order error,
The following 4-Stage Runge-kutta
method is derived.

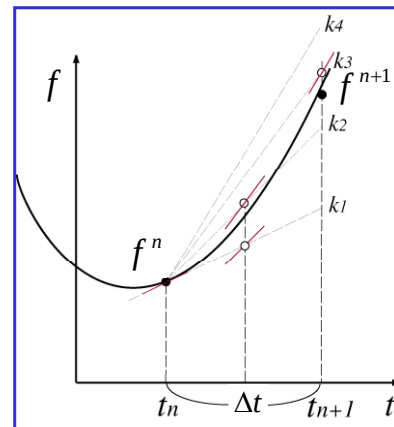
$$k_1 = \Delta t S(f^n, t^n)$$

$$k_2 = \Delta t S(f^n + 1/2k_1, t^n + 1/2\Delta t)$$

$$k_3 = \Delta t S(f^n + 1/2k_2, t^n + 1/2\Delta t)$$

$$k_4 = \Delta t S(f^n + k_3, t^n + \Delta t)$$

$$f^{n+1} = f^n + \frac{k_1 + 2k_2 + 2k_3 + k_4}{6} + \underline{O(\Delta t^5)}$$



Up to 4 stage, the stage number can reach the accuracy order.

Reference



3-stage RK Method (3rd-order accuracy)

$$k_1 = \Delta t S(f^n, t^n)$$

$$k_2 = \Delta t S(f^n + \frac{2}{3}k_1, t^n + \frac{2}{3}\Delta t)$$

$$k_3 = \Delta t S(f^n + \frac{2}{3}k_2, t^n + \frac{2}{3}\Delta t)$$

$$f^{n+1} = f^n + \frac{2k_1 + 3k_2 + 3k_3}{8} + O(\Delta t^4)$$

2D Advection Equation



$$\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} + v \frac{\partial f}{\partial y} = 0$$

Discretization : 1st-order Upwind scheme

$$\text{For } u \geq 0, \quad v \geq 0 \quad f_{i,j}^{n+1} = f_j^n - u \frac{f_{i,j}^n - f_{i-1,j}^n}{\Delta x} \Delta t - v \frac{f_{i,j}^n - f_{i,j-1}^n}{\Delta y}$$

TEST PRBLEM:

Computational Domain

$$0 \leq x \leq 1, \quad 0 \leq y \leq 1$$

Periodic Boundary Condition

$$\text{Initial Condition : } f(x, y) = \sin(k_x x) \sin(k_y y) \\ (k_x = 2\pi, \quad k_y = 2\pi)$$

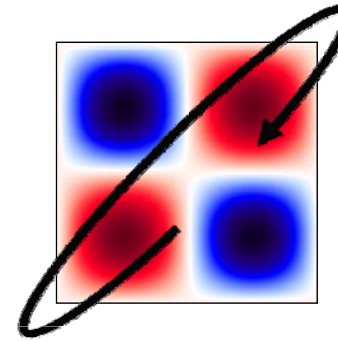
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Accuracy Check

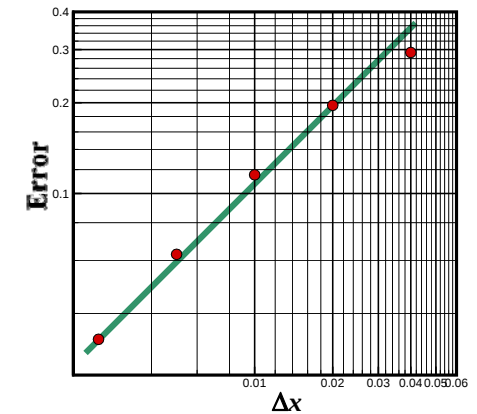


At $t = 1.0$ for $u = 1.0, \quad v = 1.0$

The profile comes back to the initial one.



Source Code



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