ODE and PDE

1 Overview

An ODE (ordinary differential equations) is an equation involving a function of a **single independent variable** and its derivatives. A PDE (partial differential equations) is an equation involving a function of **multiple independent variables** and its partial derivatives.

2 Solutions of ODEs

2.1 Euler's method (Forward Euler)

2.1.1 Derivation

Suppose we have the following equations:

$$\frac{dx}{dt} = f(x) \tag{1}$$

$$x = x(t) \tag{2}$$

Recall the **Taylor Expansion**:

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \frac{f'''(x_0)}{3!}(x - x_0)^3 + \cdots$$
(3)

Now replace f by x, x by t + h, x_0 by t:

$$x(t+h) = x(t) + h \cdot \frac{dx}{dt} + O(h^2) \tag{4}$$

Therefore, for small h:

$$\frac{dx}{dt} = \frac{x(t+h) - x(t)}{h} \tag{5}$$

The local error is $O(h^2)$, and the accumulated error over $N = \frac{1}{h}$ steps will be O(h), so this method is **1st order approx**. Now assume the input as:

$$t_0, t_1, \dots, t_n: x_0 = x(t_0)$$
 (6)

And the output as (use hat to represent prediction):

$$\hat{x}_1, \dots, \hat{x}_n: \ \hat{x}_k = x(t_k)$$
(7)

Here, k is defined from 0 to n - 1, so we have:

$$h_k = t_{k+1} - t_k \tag{8}$$

$$\hat{x}_{k+1} = \hat{x}_k + h_k \cdot f(\hat{x}_k) \tag{9}$$

2.1.2 Error Analysis

To judge whether this solution is good, we need to perform error analysis. The error consists of 3 parts:

- **Rounding Error**: the real values are stored using a finite number of digits, so the floating point arithmetic is not exact. This will affect discretization limits.
- Local Error: the difference between exact solution x_k and the computed solution \hat{x}_k . Recall that for Euler's method, we have:

$$\hat{x}_{k+1} = \hat{x}_k + h_k \cdot f(\hat{x}_k) \tag{10}$$

Now we assume \hat{x}_k is exact, so that $\hat{x}_k = x_k$, then we have:

$$\hat{x}_{k+1} = x_k + h_k \cdot f(x_k) \tag{11}$$

$$x_{k+1} - \hat{x}_{k+1} = x_{k+1} - x_k - h_k f(x_k)$$

= $h_k f(x_k) + O(h_k^2 \frac{df(x_k)}{dt}) - h_k f(x_k)$
= $O(h_k^2 \frac{df(x_k)}{dt})$

• Global Error: also start from Taylor's theorem, we have:

$$x_{k+1} - x_k = h_k f(x_k) + O(h_k^2 \frac{df(x_k)}{dt})$$
(12)

and Euler's method:

$$\hat{x}_{k+1} = \hat{x}_k + h_k \cdot f(\hat{x}_k) \tag{13}$$

Therefore we have:

$$x_{k+1} - \hat{x}_{k+1} = x_k - \hat{x}_k + h_k(f_k - \hat{f}_k) + O(h_k^2 \frac{df(x_k)}{dt})$$
(14)

Recall the mean value theorem:

$$\frac{f(b) - f(a)}{b - a} = \left. \frac{df}{dx} \right|_{x=c} \tag{15}$$

So that we have:

$$x_{k+1} - \hat{x}_{k+1} = x_k - \hat{x}_k + h_k \left. \frac{df}{dx} \right|_{x=c} \cdot (x_k - \hat{x}_k) + O(h_k^2 \frac{df(x_k)}{dt})$$
(16)

$$x_{k+1} - \hat{x}_{k+1} = (1 + h_k \left. \frac{df}{dx} \right|_{x=c}) (x_k - \hat{x}_k) + O(h_k^2 \frac{df(x_k)}{dt})$$
(17)

Here:

- 1. $(1 + h_k \frac{df}{dx}|_{x=c})$ is the **amplification factor**. Amplification occurs if $|(1 + h_k \frac{df}{dx}|_{x=c})| > 1$. If so, we say the algorithm is unstable, because error tends to magnify. However, the algorithm will be stable if $-2 < h_k \frac{df}{dx}|_{x=c} < 0$.
- 2. $O(h_k^2 \frac{df(x_k)}{dt})$ is the **local error**.
- 3. $x_k \hat{x}_k$ is the global error at t_k .
- 4. $x_{k+1} \hat{x}_{k+1}$ is the global error at t_{k+1} .

For a 2D system, $D_x f = \frac{df}{dx}$ will be a Jacobian matrix, and stability will depend on eigenvalues of $I + h_k J$ having a modulus < 1. The modulus of eigenvalues refers to the absolute value or magnitude of the eigenvalues.

2.2 Backward Euler Method

The expression of backward Euler method is shown below:

$$\hat{x}_{k+1} = \hat{x}_k + h_k f(\hat{x}_{k+1}) \tag{18}$$

Now we do the error analysis. Recall the classical taylor expansion, replace f by x, x by t, x_0 by t + h, then:

$$x(t) = x(t+h) - h \cdot \frac{dx}{dt}|_{t+h} + O(h^2)$$
(19)

Therefore, this algorithm is first order accurate, with $O(h^2)$ as **local error**. With this, we can write the true solution as:

$$x_{k+1} = x_k + h_k f_{k+1} + O(h_k^2)$$
(20)

Therefore, the **global error** could be expressed as:

$$x_{k+1} - \hat{x}_{k+1} = x_k - \hat{x}_k + h_k (f_{k+1} - \hat{f}_{k+1}) + O(h_k^2)$$
(21)

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Similarly, using mean value theorem:

$$x_{k+1} - \hat{x}_{k+1} = x_k - \hat{x}_k + h_k \left. \frac{df}{dx} \right|_{x=c} \cdot (x_{k+1} - \hat{x}_{k+1}) + O(h_k^2)$$
(22)

$$(1 - h_k \left. \frac{df}{dx} \right|_{x=c})(x_{k+1} - \hat{x}_{k+1}) = x_k - \hat{x}_k + O(h_k^2)$$
(23)

The amplification factor analysis is the same as Euler method. The algorithm is unstable when $|(1 - h_k \frac{df}{dx}|_{x=c})| > 1$, that's when $h_k \frac{df}{dx}|_{x=c} < 0$ or $h_k \frac{df}{dx}|_{x=c} > 2$

2.3 Second-Order Runge-Kutta Method (Midpoint Method)

2.3.1 Definition

Assume an ODE as $\frac{dy}{dt} = f(t, y)$, with initial condition $y(t_0) = y_0$ and a step size h. Then, for n = 0, 1, 2, ...:

- 1. Calculate $k_1 = hf(t_n, y_n)$.
- 2. Calculate $\hat{y}_{mid}=\hat{y}_{n+\frac{1}{2}}=y_n+\frac{1}{2}k_1$
- 3. Calculate $\hat{k}_2 = hf(t_n + \frac{h}{2}, \hat{y}_{mid})$
- 4. Update $\hat{y}_{n+1} = y_n + \hat{k}_2$
- 5. Update $t_{n+1} = t_n + h$

2.3.2 Second Order Proof

For each step of the algorithm:

1. Based on the definition of f (here, we assume y_n is exact, so k_1 is also exact):

$$k_1 = hf(t_n, y_n) = hy'(t_n)$$
 (24)

2. Now plug this into the midpoint expression:

$$\hat{y}_{mid} = \hat{y}_{n+\frac{1}{2}} = y_n + \frac{h}{2}y'(t_n) \tag{25}$$

Recall the taylor expansion, the exact value is (this may not be used, just showing):

$$y_{n+\frac{1}{2}} = y(t_n + \frac{1}{2}h) = y(t_n) + \frac{h}{2} \cdot \frac{dy}{dt} + O(h^2)$$
(26)

3. The calculated k_2 could be expressed as:

$$\hat{k}_2 = hf(t_n + \frac{h}{2}, \hat{y}_{mid}) = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}y'(t_n))$$
(27)

Because f is a function of both y and t, the approximation will be:

$$f(t_n + \frac{h}{2}, \hat{y}_{mid}) = f(t_n, y_n) + \frac{h}{2}f'(t_n, y_n) = y'(t_n) + \frac{h}{2}(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial y}y'(t_n))$$
(28)

Therefore:

$$\hat{k}_2 = h[y'(t_n) + \frac{h}{2}(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial y}y'(t_n))]$$
(29)

4. Finally, the calculated y_{n+1} :

$$\hat{y}_{n+1} = y_n + \hat{k}_2 = y_n + hy'(t_n) + \frac{h^2}{2}\left(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial y}y'(t_n)\right)$$
(30)

Recall the taylor expansion of y, we have:

$$y_{n+1} = y(t_n + h) = y(t_n) + hy'(t_n) + \frac{h}{2}y''(t_n) + O(h^3)$$
(31)

Notice that:

$$f(t_n, y_n) = y'(t_n) \tag{32}$$

So we have:

$$y''(t_n) = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y}y'(t_n)$$
(33)

Therefore, the local truncation error of RK2 method is (at each step):

$$y_{n+1} - \hat{y}_{n+1} = O(h^3) \tag{34}$$

And the global truncation error which is accumulated over $N = \frac{1}{h}$ steps will be $O(h^2)$. Therefore, RK2 method is in second-order.

3 Macroscopic Models of Traffic Flow (PDE)

3.1 Overview

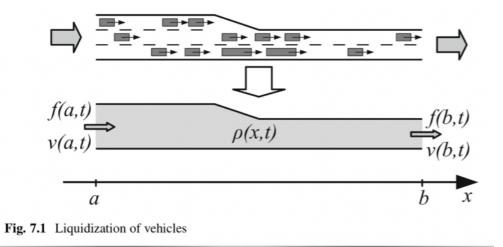


Figure 1: Traffic Flow

In this problem, we want to use PDE system with respect to space (x) and time (t) to model the traffic flow. Some basic definitions include:

- v(x,t): speed of vehicles at (x,t), with unit as [distance]/[time]
- $\rho(x,t)$: density of vehicles, with unit as [#cars]/[distance]
- f(x,t): traffic flow, with unit as [#cars]/[time]

Let ρ_{max} be the bumper-to-bumper traffic density and v_{max} , then we have:

$$0 \le \rho(x, t) \le \rho_{max} \tag{35}$$

$$0 \le v(x,t) \le v_{max} \tag{36}$$

3.2 Model 0: Homogeneous Flow

Assume there is no dependence on (x, t), then we have:

$$\rho(x,t) = \bar{\rho}, \quad v(x,t) = \bar{v}, \quad f(x,t) = \bar{f}$$
(37)

And assume the final time as τ , so the total number of cars will be:

$$\#cars = \frac{[\#cars]}{[dist]} \cdot \frac{[dist]}{[time]} \cdot time = \bar{\rho}\bar{v}\tau$$
(38)

So the number of cars passing a point at τ will be:

$$\frac{\bar{\rho}\bar{v}\tau}{\tau} = \bar{\rho}\bar{v} = \bar{f} \tag{39}$$

3.3 Model 1: Speed Depends on Density

Based on intuition, if there are more cars, the speed will decrease. In other words, $\rho \to 0$ when $v \to v_{max}$ and $\rho \to \rho_{max}$ when $v \to 0$. Assume this relation is linear then:

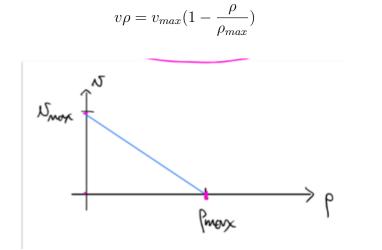


Figure 2: Linear Relation

So the traffic flow will be:

$$f = f(\rho) = \rho \cdot v(\rho) = v_{max}\rho(1 - \frac{\rho}{\rho_{max}})$$
(41)

In order to simplify the model, we could use non-dimensional form:

$$\hat{\rho} = \frac{\rho}{\rho_{max}} \tag{42}$$

$$\hat{f} = \frac{f}{\rho_{max} v_{max}} \tag{43}$$

Then change the previous expression to:

$$\rho_{\max} v_{\max} \hat{f} = v_{\max} \rho_{\max} \hat{\rho} (1 - \hat{\rho}) \tag{44}$$

$$\hat{f}(\hat{\rho}) = \hat{\rho}(1-\hat{\rho}) \tag{45}$$

Now we can define the non-dimensional v as:

$$\hat{v} = \frac{\hat{f}}{\hat{\rho}} = 1 - \hat{\rho} \tag{46}$$

Therefore, the max flow occurs when $\hat{\rho} = \frac{1}{2}$, and so:

$$\hat{f}(\frac{1}{2}) = \frac{1}{4} \tag{47}$$

$$f \le \frac{\rho_{max} v_{max}}{4} \tag{48}$$

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(40)

3.4 Model 2: Inhomogeneous Flow

In this model, density varies in space $\rho = \rho(x, t)$. Let n(t) be the number of cars between x = a and x = b at time t, then:

$$\frac{dn}{dt} = \int_{a}^{b} \frac{\partial \rho}{\partial t} dx \tag{49}$$

Also assume no on/off ramps, so no cars are lost. Then the change in n(t) is also the difference in flow at the endpoints:

$$\frac{dn}{dt} = f(a,t) - f(b,t) = -\int_{a}^{b} \frac{\partial f}{\partial x} dx$$
(50)

Combine these two equations we have:

$$\frac{dn}{dt} = \int_{a}^{b} \left(\frac{\partial\rho}{\partial t} + \frac{\partial f}{\partial x}\right) dx = 0$$
(51)

Because this equation should fit the general case, so must be true for all a, b, t, so we could get the continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial f}{\partial x} = 0 \tag{52}$$

Assume drivers react instantaneously to changes in density, so:

$$f = f(\rho) \tag{53}$$

4 Solutions of PDEs

4.1 Discretization

First we need to discretize space and time uniformly:

$$x_i \in \{0, l, 2l, \ldots\} \tag{54}$$

$$t_j \in \{0, h, 2h, \ldots\} \tag{55}$$

4.2 First Order Forward Finite Difference Approximation (Upwind)

4.2.1 Definition

The first order forward finite difference approximation could (also called upwind method) be expressed as:

$$\frac{\partial f}{\partial x} \approx \frac{f(x+l,t) - f(x,t)}{l} = \frac{f(x_{i+1},t_j) - f(x_i,t_j)}{l} \tag{56}$$

$$\frac{\partial \rho}{\partial t} \approx \frac{\rho(x, t+h) - \rho(x, t)}{h} = \frac{\rho(x_i, t_{j+1}) - \rho(x_i, t_j)}{h}$$
(57)

Here, we define:

$$f_{i,j} = f(x_i, t_j), \ \ \rho_{i,j} = \rho(x_i, t_j)$$
 (58)

Therefore, the **continuity equation** could be expressed as:

$$\frac{\rho_{i,j+1} - \rho_{i,j}}{h} + \frac{f_{i+1,j} - f_{i,j}}{l} = 0$$
(59)

And the **logistic flow model** could be expressed as:

$$f_{i,j} = v_{max}\rho_{i,j}\left(1 - \frac{\rho_{i,j}}{\rho_{max}}\right) \tag{60}$$

Now plug the logistic flow model into the continuity equation:

$$\frac{\rho_{i,j+1} - \rho_{i,j}}{h} + \frac{v_{\max}}{l} \left[\rho_{i+1,j} \left(1 - \frac{\rho_{i+1,j}}{\rho_{\max}} \right) - \rho_{i,j} \left(1 - \frac{\rho_{i,j}}{\rho_{\max}} \right) \right]$$
(61)

Rearrange, we could get the density solution:

$$\rho_{i,j+1} = \rho_{i,j} - \frac{h}{l} v_{\max} \left[\rho_{i+1,j} \left(1 - \frac{\rho_{i+1,j}}{\rho_{\max}} \right) - \rho_{i,j} \left(1 - \frac{\rho_{i,j}}{\rho_{\max}} \right) \right]$$
(62)

4.2.2 Accuracy and Stability Analysis

Rearrange the continuity equation, we get:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial f}{\partial x} = -\frac{df}{d\rho} \frac{\partial \rho}{\partial x}$$
(63)

If we consider a simpler, linear system (ρ as u):

$$\frac{\partial u}{\partial t} = c \frac{\partial u}{\partial x} \tag{64}$$

Here we define:

$$u = u(x, t), \ u_0(x) = u(x, 0)$$
 (65)

Assume the traveling wave moving at velocity c, then:

$$u(x,t) = u_0(x+ct)$$
 (66)

This could be proved. Assume y = x + ct, then:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial t} u_0(x+ct) = \left. \frac{du_0}{dy} \right|_{y=x+ct} \cdot \frac{\partial y}{\partial t} = c \left. \frac{du_0}{dy} \right|_{y=x+ct}$$
(67)

$$c\frac{du}{dx} = c\frac{\partial}{\partial x}u_0(x+ct) = c\left.\frac{du_0}{dy}\right|_{y=x+ct} \cdot \frac{\partial y}{\partial x} = c\left.\frac{du_0}{dy}\right|_{y=x+ct}$$
(68)

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By intuition, the stability depends on time step (h), spatial step (s) and wave speed (c). Consider the true solution at some point x, then after j time steps, it moves a distance cjh. For stability, we need to ensure that **information does not travel more than one spatial grid cell in one time step**. In math:

$$cjh \le js$$
 (69)

$$c\frac{h}{s} \le 1 \tag{70}$$

Here we define c_s^h as the CFL (Courant-Friedrichs-Lewy) number, or Courant number. This is a necessary condition for stability, but not sufficient condition.

Now for accuracy, we first rewrite the simplified wave equation:

$$\frac{u(x,t+h) - u(x,t)}{h} = c \frac{u(x+s,t) - u(x,t)}{s}$$
(71)

Recall the taylor expansion:

$$u(x,t+h) = u(x,t) + h\frac{\partial u}{\partial t} + \frac{h^2}{2}\frac{\partial^2 u}{\partial t^2} + O(h^3)$$
(72)

$$u(x+s,t) = u(x,t) + s\frac{\partial u}{\partial x} + \frac{s^2}{2}\frac{\partial^2 u}{\partial x^2} + O(h^3)$$
(73)

Plug these into the wave equation, we have:

$$\frac{\partial u}{\partial t} + \frac{h}{2}\frac{\partial^2 u}{\partial t^2} + O(h^2) = c\frac{\partial u}{\partial x} + \frac{cs}{2}\frac{\partial^2 u}{\partial x^2} + O(s^2)$$
(74)

Notice that $\frac{\partial u}{\partial t} = c \frac{\partial u}{\partial x}$, so the first different terms are O(h) and O(s), and the truncation error terms are $O(h^2)$ and $O(s^2)$. After integration over steps, we know that this method is **first order accurate in** h **and** s.

From the wave equation, we also know that:

$$\frac{\partial^2 u}{\partial t^2} = c \frac{\partial^2 u}{\partial t \partial x} = c \frac{\partial}{\partial x} \frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2}$$
(75)

Therefore, when:

$$\frac{h}{2}\frac{\partial^2 u}{\partial t^2} = \frac{hc^2}{2}\frac{\partial^2 u}{\partial x^2} = \frac{cs}{2}\frac{\partial^2 u}{\partial x^2}$$
(76)

or in other words:

$$s = ch \tag{77}$$

the first different terms will be $O(h^2)$ and $O(s^2)$, then accuracy would be second order.

4.3 Second Order Forward Finite Difference Approximation (Lax-Wendroff Method)

4.3.1 Definition

After investigation of first order method, now we want to improve the accuracy to second order. The expression is:

$$\frac{u_{i,j+1} - u_{i,j}}{h} = c \frac{u_{i+1,j} - u_{i-1,j}}{2s} + c^2 \frac{h}{2} \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{s^2}$$
(78)

4.3.2 Accuracy Analysis

Recall the Taylor expansion in first order method:

$$\frac{u_{i,j+1} - u_{i,j}}{h} = \frac{\partial u}{\partial t} + \frac{h}{2}\frac{\partial^2 u}{\partial t^2} + O(h^2)$$
(79)

For the spatial derivative, we define (g is only a function of x, u is a function of xand t, will change g back to u):

$$(a): g(x+s) = g(x) + s\frac{dg}{dx} + \frac{s^2}{2}\frac{d^2g}{dx^2} + O(s^3)$$
(80)

$$(b): g(x-s) = g(x) - s\frac{dg}{dx} + \frac{s^2}{2}\frac{d^2g}{dx^2} + O(s^3)$$
(81)

Therefore, we have:

$$\frac{g(x+s) - g(x-s)}{2s} = \frac{dg}{dx} + O(s^2)$$
(82)

$$g(x+s) + g(x-s) = 2g(x) + s^2 \frac{d^2g}{dx^2} + O(s^3)$$
(83)

$$\frac{g(x+s) - 2g(x) + g(x-s)}{s^2} = \frac{d^2g}{dx^2} + O(s)$$
(84)

Also recall the first order method:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \tag{85}$$

Change g back to u, we have:

$$\frac{\partial u}{\partial t} + \frac{h}{2}\frac{\partial^2 u}{\partial t^2} + O(h^2) = c\frac{\partial u}{\partial x} + O(s^2) + c^2\frac{h}{2}\frac{\partial^2 u}{\partial x^2} + O(hs)$$
(86)

$$\frac{\partial u}{\partial t} = c \frac{\partial u}{\partial x} + O(h^2 + s^2 + hs) \tag{87}$$

Because the first different terms are $O(h^2)$ and $O(s^2)$, so this method is second order accuracy.

4.3.3 Stability Analysis

Recall that in ODE stability analysis, for Euler method we have:

$$x_{k+1} - \hat{x}_{k+1} = (1 + h_k \left. \frac{df}{dx} \right|_{x=c}) (x_k - \hat{x}_k) + O(h_k^2 \frac{df(x_k)}{dt})$$
(88)

Before, we define $(1 + h_k \frac{df}{dx}|_{x=c})$ as the amplification factor. In von Neumann stability analysis, this is defined as **growth factor**. Because here the growth factor is derived from the numerical scheme, so it is denoted as \hat{G} . Define $x_k - \hat{x}_k$ as Δ_k , because of the existence of local error, we have the following relationship:

$$\Delta_{k+1} \le \hat{G}\Delta_k \le \hat{G}^2 \Delta_{k-1} \le \dots \le \hat{G}^k \Delta_1 \tag{89}$$

To get converging solution, we want the error at each step is decreasing or at least staying the same. Therefore we want $|\hat{G}| \leq 1$ for stability.

Now recall the PDE wave function, do the Fourier transfer, we have:

$$u_0(x) = e^{i\lambda x} \tag{90}$$

$$u(x,t) = u_0(x+ct) = e^{i\lambda(x+ct)} = e^{i\lambda ct} \cdot e^{i\lambda x} = e^{i\lambda ct} \cdot u_0(x)$$
(91)

Here, we define the **exact growth factor (not from numerical scheme)** $G = e^{i\lambda ct}$. The actual growth factor \hat{G} will depend on the numerical method we choose. Take upwind method as an example. Assume the CFL number as $r = \frac{ch}{s}$, then:

$$u(x,t+h) = u(x,t) + r \left[u(x+s,t) - u(x,t) \right]$$
(92)

$$u(x,t+h) = (1-r)u(x,t) + ru(x+s,t)$$
(93)

Similarly, assume $u(x, 0) = e^{i\lambda x}$, so after one time step h:

$$u(x,h) = (1-r)e^{i\lambda x} + re^{i\lambda(x+s)}$$
(94)

$$u(x,h) = (1 - r + re^{i\lambda s})e^{i\lambda x}$$
(95)

Therefore we could define the actual growth factor as:

$$\hat{G} = 1 - r + re^{i\lambda s} \tag{96}$$

Expand the exponential term:

$$\hat{G} = (1-r) + r + r(i\lambda s) + r(i\lambda s)^2/2 + \cdots$$
 (97)

$$\hat{G} = 1 + i\lambda rs + r(i\lambda s)^2/2 + \cdots$$
(98)

And the exact growth factor at the first time step will be:

$$G = e^{i\lambda ch} = e^{i\lambda rs} \tag{99}$$

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Also expand the exponential term:

$$G = 1 + i\lambda rs + \frac{(i\lambda rs)^2}{2} + \cdots$$
(100)

From the observation, when $r = r^2 = 1$, or unit CFL number, we have $\hat{G} \approx G$. And for upwind method, \hat{G} matches with G in first order. For Lax-Wendroff method, we have:

$$\hat{G} = (1 - r^2) + \frac{1}{2}(r^2 + r)e^{i\lambda s} + \frac{1}{2}(r^2 - r)e^{-i\lambda s}$$
(101)

Expand the exponential term:

$$\hat{G} = 1 + r(i\lambda s) + r^2(i\lambda s)^2/2 + O((\lambda s)^3)$$
(102)

Therefore, this \hat{G} matches G in second order.

4.4 Diffusion Process Growth Factor

Assume a simple diffusion model:

$$\frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2} \tag{103}$$

Assume a general solution:

$$u(x,t) = G(t)e^{i\lambda x}$$
(104)

Therefore:

$$\frac{\partial u}{\partial t} = \frac{dG}{dt}e^{i\lambda x} \tag{105}$$

$$\frac{\partial u}{\partial x} = G(t) \cdot (i\lambda) \exp(i\lambda x) \tag{106}$$

$$\frac{\partial^2 u}{\partial x^2} = -\lambda^2 G(t) \exp(i\lambda x) \tag{107}$$

Rearrange the equations, we have:

$$\frac{dG}{dt} = -(c\lambda)^2 G \tag{108}$$

$$G \sim \exp(-c^2 \lambda^2 t) \tag{109}$$

5 Numerical Method (PDE) Summary

5.1 Overview

Before the start of summary, several definitions need to be clarified.

- 1. **Explicit**: explicit methods compute the solution at the next time step directly from the known information at the current time step. They do not require solving any linear or nonlinear system of equations.
- 2. **Implicit**: implicit methods compute the solution at the next time step by solving an equation that involves **both the current and the next time steps**. This generally requires solving a system of linear or nonlinear equations.
- 3. Conditionally Stable: stability depends on the choice of the time step Δt and spatial step Δx . The method is stable only if these parameters satisfy certain conditions or constraints.
- 4. Unconditionally Stable: the method is stable for any choice of the time step Δt and spatial step Δx .

For the following method, we use heat equation as the example if no specification:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \tag{110}$$

5.2 Forward Euler Method (Forward Time Centered Space, FTCS)

5.2.1 Definition

Time derivative discretization:

$$\frac{\partial u}{\partial t} \approx \frac{u_j^{n+1} - u_j^n}{\Delta t} \tag{111}$$

Space derivative discretization:

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}$$
(112)

Solution:

$$u_{j}^{n+1} = u_{j}^{n} + \alpha \Delta t \frac{u_{j+1}^{n} - 2u_{j}^{n} + u_{j-1}^{n}}{(\Delta x)^{2}}$$
(113)

5.2.2 Analysis

Because the solution does not contain the next time steps variable, so this method is **explicit**. This method is **conditionally stable**, for the heat equation, the stability criterion is:

$$\Delta t \le \frac{(\Delta x)^2}{2\alpha} \tag{114}$$

5.3 Backward Euler Method

5.3.1 Definition

Time derivative discretization:

$$\frac{\partial u}{\partial t} \approx \frac{u_j^{n+1} - u_j^n}{\Delta t} \tag{115}$$

Space derivative discretization:

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\Delta x)^2}$$
(116)

Solution:

$$u_j^{n+1} = u_j^n + \alpha \Delta t \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\Delta x)^2}$$
(117)

5.3.2 Analysis

This method takes the next time step variable, so it is **implicit**. This method is **unconditionally stable**.

5.4 Upwind Solution

5.4.1 Definition

Upwind method is commonly used for solving **hyperbolic PDE**. Consider the 1D linear advection equation:

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0 \tag{118}$$

Here c is the wave speed, which could be positive or negative. The time derivative discretization is:

$$\frac{\partial u}{\partial t} \approx \frac{u_j^{n+1} - u_j^n}{\Delta t} \tag{119}$$

When c > 0, the space discretization will use the backward difference:

$$\frac{\partial u}{\partial x} \approx \frac{u_j - u_{j-1}}{\Delta x} \tag{120}$$

And the solution will be:

$$u_{j}^{n+1} = u_{j}^{n} - \frac{c\Delta t}{\Delta x} (u_{j}^{n} - u_{j-1}^{n})$$
(121)

When c < 0, the space discretization will use forward difference:

$$\frac{\partial u}{\partial x} \approx \frac{u_{j+1} - u_j}{\Delta x} \tag{122}$$

And the solution will be:

$$u_{j}^{n+1} = u_{j}^{n} - \frac{c\Delta t}{\Delta x} (u_{j+1}^{n} - u_{j}^{n})$$
(123)

5.4.2 Analysis

This method is **explicit** and **conditionally stable**. The stability criterion is typically given by the CFL condition:

$$\left|\frac{c\Delta t}{\Delta x}\right| \le 1\tag{124}$$

5.5 Lax-Wendroff Method

5.5.1 Definition

Lax-Wendroff method is also commonly used for solving hyperbolic PDE. Consider the 1D linear advection equation:

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0 \tag{125}$$

First we do the Taylor expansion of u in time around t^n :

$$u_j^{n+1} = u_j^n + \Delta t \frac{\partial u_j^n}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 u_j^n}{\partial t^2} + O(\Delta t^3)$$
(126)

Recall the previous chapter, we have:

$$\frac{\partial u}{\partial t} = -c \frac{\partial u}{\partial x} \tag{127}$$

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \tag{128}$$

So the expansion now becomes:

$$u_j^{n+1} = u_j^n - c\Delta t \frac{\partial u_j^n}{\partial x} + \frac{c^2 \Delta t^2}{2} \frac{\partial^2 u_j^n}{\partial x^2} + O(\Delta t^3)$$
(129)

Now approximate the first and second spatial derivatives using central differences:

$$\frac{\partial u_j^n}{\partial x} \approx \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} \tag{130}$$

$$\frac{\partial^2 u_j^n}{\partial x^2} \approx \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} \tag{131}$$

The final solution will be:

$$u_{j}^{n+1} = u_{j}^{n} - \frac{c\Delta t}{2\Delta x} (u_{j+1}^{n} - u_{j-1}^{n}) + \frac{c^{2}\Delta t^{2}}{2(\Delta x)^{2}} (u_{j+1}^{n} - 2u_{j}^{n} + u_{j-1}^{n})$$
(132)

5.5.2 Analysis

This method is **explicit** and **conditionally stable**. The stability criterion is given by the CFL condition:

$$\left|\frac{c\Delta t}{\Delta x}\right| \le 1\tag{133}$$