

Schwartz class $S(\mathbb{R}^n)$ consists of functions $f \in C^\infty(\mathbb{R}^n)$ such that for any pair of multiindices α, β :

$$p_{\alpha\beta}(f) := \sup_x |x^\alpha D^\beta f(x)| < +\infty$$

where

$$\alpha = (\alpha_1, \dots, \alpha_n), \quad \beta = (\beta_1, \dots, \beta_n) \quad [\text{multi-index}]$$

and

$$x^\alpha = x_1^{\alpha_1} \dots x_n^{\alpha_n} \quad D^\beta f(x) = \frac{\partial^{|\beta|}}{\partial x_1^{\beta_1} \dots \partial x_n^{\beta_n}} f(x).$$

$$|\beta| = \sum_{i=1}^n \beta_i = \text{order of derivative.}$$

Example:

$$n=2, \quad \beta = (1, 2)$$

$$D^\beta f(x) = \frac{\partial^3}{\partial x_1 \partial x_2^2} f(x).$$

* If $f \in S(\mathbb{R}^n)$, then f is infinitely differentiable and rapidly decreasing.
- Every derivative of f goes to zero faster than any polynomial.

$$C_c^\infty(\mathbb{R}^n) \subset S(\mathbb{R}^n) \subset C^\infty(\mathbb{R}^n).$$

Fourier Transform: Let $f \in L^1(\mathbb{R}^n) = \{f: \mathbb{R}^n \rightarrow \mathbb{R} \mid \int_{\mathbb{R}^n} |f| < +\infty\}$ function,

then the Fourier Transform of f is:

$$\widehat{f}(\xi; f) = \widehat{f}(\xi) = \int_{\mathbb{R}^n} f(x) e^{-2\pi i x \cdot \xi} dx.$$

Proposition: For $f \in L^1(\mathbb{R}^n)$,

$$|\widehat{f}(\xi)| \leq \int_{\mathbb{R}^n} |f(x)| dx < +\infty.$$

Proof:

$$|\widehat{f}(\xi)| \leq \int_{\mathbb{R}^n} |f(x) e^{-2\pi i x \cdot \xi}| dx \leq \int_{\mathbb{R}^n} |f(x)| dx < +\infty.$$

\uparrow \mathbb{R}^n \uparrow
 $|e^{i\alpha}| = 1$ $f \in L^1(\mathbb{R})$

Properties of Fourier Transform:

- Let $f, g \in S(\mathbb{R}^n)$, then

$$(1) \text{ F.T. is linear: } \widehat{f+g} = \widehat{f} + \widehat{g}$$

$$(i) \hat{f}(\xi) \in S(\mathbb{R}^n)$$

$$(ii) \frac{\partial \hat{f}}{\partial x_j}(\xi) = 2\pi i \xi_j \hat{f}(\xi) \quad \text{and} \quad (-2\pi i)(\widehat{x_j f})(\xi) = \frac{\partial \hat{f}}{\partial \xi_j}(\xi).$$

$$(iii) \int_{\mathbb{R}^n} f(x) \hat{g}(x) dx = \int_{\mathbb{R}^n} \hat{f}(x) g(x) dx.$$

$$(iv) \text{ Inversion formula: } f(x) = \int_{\mathbb{R}^n} \hat{f}(\xi) e^{2\pi i x \cdot \xi} d\xi.$$

$$(v) \text{ If } f(x) = e^{-\pi|x|^2}, \text{ then } \hat{f}(x) = f(x).$$

Proof: (i), (iv) skip

$$\begin{aligned} (ii) (a) \frac{\partial \hat{f}}{\partial \xi_j}(\xi) &= \int_{\mathbb{R}^n} \frac{\partial f}{\partial x_j}(x) e^{-2\pi i \xi \cdot x} dx = \int_{\mathbb{R}^n} \left[\frac{\partial}{\partial x_j} (f(x) e^{-2\pi i \xi \cdot x}) - f(x) (-2\pi i \xi_j) e^{-2\pi i \xi \cdot x} \right] dx \\ &= \lim_{r \rightarrow \infty} \int_{\partial B_r(0)} f(x) e^{-2\pi i \xi \cdot x} n_j d\Gamma + 2\pi i \xi_j \int_{\mathbb{R}^n} f(x) e^{-2\pi i \xi \cdot x} dx \\ &= 2\pi i \xi_j \hat{f}(\xi). \quad \square \end{aligned}$$

$$\begin{aligned} (b) \frac{\partial \hat{f}}{\partial \xi_j}(\xi) &= \frac{\partial}{\partial \xi_j} \int_{\mathbb{R}^n} f(x) e^{-2\pi i \xi \cdot x} dx = \int_{\mathbb{R}^n} f(x) (-2\pi i x_j) e^{-2\pi i \xi \cdot x} dx \\ &= (-2\pi i) (\widehat{x_j f})(\xi). \end{aligned}$$

$$(v) f(x) = e^{-\pi|x|^2} = e^{-\pi x_1^2} \dots e^{-\pi x_n^2}.$$

Sufficient to prove for $n=1$, because if $\widehat{e^{-\pi x_i^2}} = e^{-\pi \xi_i^2}$, then

$$\begin{aligned} \widehat{e^{-\pi|x|^2}} &= \widehat{e^{-\pi x_1^2} \dots e^{-\pi x_n^2}} = \int e^{-\pi x_1^2} \dots e^{-\pi x_n^2} e^{-2\pi i x_1 \xi_1} \dots e^{-2\pi i x_n \xi_n} dx_1 \dots dx_n \\ &= \int e^{-\pi x_1^2} e^{-2\pi i x_1 \xi_1} dx_1 \dots \int e^{-\pi x_n^2} e^{-2\pi i x_n \xi_n} dx_n \\ &= \widehat{e^{-\pi x_1^2}} \dots \widehat{e^{-\pi x_n^2}} = e^{-\pi|\xi|^2}. \end{aligned}$$

Let $x, \xi \in \mathbb{R}$:

$$\begin{aligned} \widehat{e^{-\pi x^2}} &= \int_{\mathbb{R}} e^{-\pi x^2} e^{-2\pi i \xi x} dx = \int_{\mathbb{R}} e^{-\pi x^2} e^{-2\pi i \xi x} e^{-\pi \xi^2} e^{\pi \xi^2} dx \\ &= e^{-\pi \xi^2} \int_{\mathbb{R}} e^{-\pi(x^2 + 2i\xi x - \xi^2)} dx \\ &= e^{-\pi \xi^2} \int_{\mathbb{R}} e^{-\pi(x+i\xi)^2} dx \\ &= e^{-\pi \xi^2} \int_{\mathbb{R}} e^{-\pi y^2} dy = e^{-\pi \xi^2}. \quad \square \end{aligned}$$

$$\begin{aligned}
 \text{(iii)} \quad \int_{\mathbb{R}^n} f(x) \hat{g}(x) dx &= \int_{\mathbb{R}^n} f(x) \int_{\mathbb{R}^n} g(z) e^{-2\pi i z \cdot x} dz dx \\
 &= \iint_{\mathbb{R}^n} f(x) g(z) e^{-2\pi i z \cdot x} dz dx, \text{ Fubini b/c both } f, g \in S(\mathbb{R}^n) \\
 &= \iint_{\mathbb{R}^n} f(x) g(z) e^{-2\pi i z \cdot x} dx dz \\
 &= \int_{\mathbb{R}^n} g(z) \int_{\mathbb{R}^n} f(x) e^{-2\pi i z \cdot x} dx dz \\
 &= \int_{\mathbb{R}^n} g(z) \hat{f}(z) dz, \text{ change of variables} \\
 &= \int_{\mathbb{R}^n} \hat{f}(x) g(x) dx
 \end{aligned}$$

□

Examples

Problem 6, Hwk 4

Let $u(t, x)$ satisfy the heat equation, $u_t - \Delta u = 0$, $t > 0$, $x \in \mathbb{R}^n$ (*)
with IC: $u(0, x) = f(x)$

(a) Use F.T. to show $u(t, x) = \int e^{2\pi i \xi \cdot x - 4\pi^2 |\xi|^2 t} \hat{f}(\xi) d\xi$

(b) Convert answer in (a) to the form $u(t, x) = \int G(t, x-y) f(y) dy$.

Solution:

(a) Take F.T. in x of (*)

$$\begin{aligned}
 \widehat{\Delta u} &= \sum_{k=1}^n \frac{\partial^2 u}{\partial x_k^2} = \sum_{k=1}^n \frac{\partial}{\partial x_k} \left(\frac{\partial u}{\partial x_k} \right) = \sum_{k=1}^n 2\pi i \xi_k \frac{\partial u}{\partial x_k} = \sum_{k=1}^n (-4\pi^2) \xi_k^2 \hat{u}(\xi) \\
 &\quad \uparrow \\
 &\quad \text{linearity} \\
 &= (-4\pi^2) |\xi|^2 \hat{u}(\xi)
 \end{aligned}$$

$$\begin{aligned}
 \Rightarrow \hat{u}_t &= -4\pi^2 |\xi|^2 \hat{u}(t, \xi) \xrightarrow{\text{solve ODE}} \hat{u}(t, \xi) = \hat{u}(0, \xi) e^{-4\pi^2 |\xi|^2 t} \\
 \hat{u}(0, \xi) &= \hat{f} \quad \quad \quad = \hat{f}(\xi) e^{-4\pi^2 |\xi|^2 t}
 \end{aligned}$$

Inverse F.T.:

$$u(t, x) = \int_{\mathbb{R}^n} \hat{u}(t, \xi) e^{2\pi i \xi \cdot x} d\xi = \int_{\mathbb{R}^n} e^{2\pi i \xi \cdot x - 4\pi^2 |\xi|^2 t} \hat{f}(\xi) d\xi$$

(b) $u(t, x) = \int_{\mathbb{R}^n} e^{2\pi i \xi \cdot x} e^{-4\pi^2 |\xi|^2 t} \int_{\mathbb{R}^n} f(y) e^{-2\pi i \xi \cdot y} dy d\xi$ combine integrals
use Fubini

$$= \iint_{\mathbb{R}^n} f(y) e^{2\pi i \xi \cdot (x-y)} e^{-4\pi^2 |\xi|^2 t} d\xi dy, \text{ change of variables: } \xi \rightarrow \frac{\xi}{\sqrt{4\pi t}}$$

$$= \int_{\mathbb{R}^n} f(y) \int_{\mathbb{R}^n} e^{-\pi |\xi|^2} e^{2\pi i \frac{\xi \cdot (x-y)}{\sqrt{4\pi t}}} \frac{d\xi}{(4\pi t)^{n/2}} dy$$

$$= \int_{\mathbb{R}^n} f(y) e^{-\pi \frac{|x-y|^2}{4\pi t}} \frac{1}{(4\pi t)^{n/2}} dy = \int_{\mathbb{R}^n} \frac{1}{(4\pi t)^{n/2}} e^{-\frac{|x-y|^2}{4t}} f(y) dy$$

□

Introduction to Numerical PDEs

- Background: Taylor's Theorem, O notation
- Finite Differences Approximations
- Aside: ODE solvers (implicit vs. explicit)
- Truncation error, consistency, convergence
- Ex: KdV equation

Background: Taylor's Theorem.

Let $k \geq 1$ integer and $f: \mathbb{R} \rightarrow \mathbb{R}$ $k+1$ times differentiable at $a \in \mathbb{R}$. Then, $\exists h_0 > 0$ such that

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \dots + \frac{f^{(k)}(a)}{k!}(x-a)^k + \frac{f^{(k+1)}(\xi)}{(k+1)!}(x-a)^{k+1}$$

for $\xi \in [a, x]$.

$$R_k(x) = \frac{f^{(k+1)}(\xi)}{(k+1)!}(x-a)^{k+1} = O((x-a)^{k+1})$$

O -notation: $f(x) = O(g(x))$ as $x \rightarrow a$ iff $\exists M, \delta > 0$ such that

$$|f(x)| \leq M|g(x)| \text{ for } |x-a| < \delta.$$

* as $x \rightarrow a$, f can be bounded by a constant times g .

Finite Differences Approximations

Consider a function $f \in \mathbb{R}$, sufficiently smooth (if I need a derivative, I have it).

Taylor series about x , to first order.

$$f(x+h) = f(x) + f'(x)h + \frac{h^2}{2}f''(\xi) \Rightarrow f'(x) = \frac{f(x+h) - f(x)}{h} + O(h).$$

$$\text{Similarly, } f'(x) = \frac{f(x) - f(x-h)}{h} + O(h)$$

as $h \rightarrow 0$
(for a given x , $\frac{1}{2}f''(\xi)$ constant)

$$f(x+h) = f(x) + f'(x)h + \frac{h^2}{2}f''(x) + \frac{h^3}{3!}f'''(x) + O(h^4)$$

$$f(x-h) = f(x) - f'(x)h + \frac{h^2}{2}f''(x) - \frac{h^3}{3!}f'''(x) + O(h^4)$$

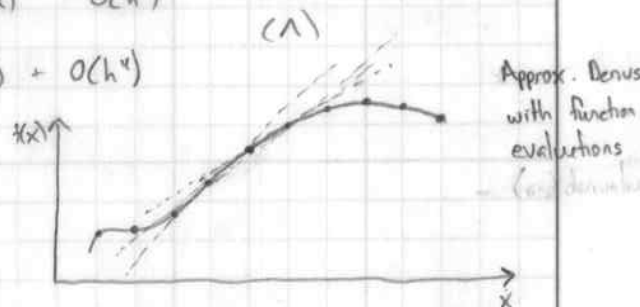
$$\Rightarrow f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

Method of Undetermined Coefficients

Ex: One-sided approx. to $f'(x)$ @ equally spaced points: $x, x-h, x-2h$

$$D_2 f(x) = a f(x) + b f(x-h) + c f(x-2h).$$

$$= a f(x) + b [f(x) - f'(x)h + \frac{h^2}{2}f''(x) - \frac{f'''(x)h^3}{3!} + O(h^4)] + c [f(x) - f'(x)2h + \frac{4h^2}{2!}f''(x) - \frac{f'''(x)8h^3}{3!} + O(h^4)]$$



* fit polynomial to f at a certain point - evaluate the derivative of the polynomial @ the point of interest.

1st order approx. to 1st derivatives

2nd order approx. to 2nd derivatives

Deriving finite difference approx

$$= f(x)[a+b+c] + f'(x)[-bh-2ch] + f''(x)\left[\frac{h^2}{2!}b + 2h^2c\right] + f'''(x)\left[\frac{h^3}{3!}b + \frac{4}{3}h^3c\right] + \dots$$

For $D_2 f$ to agree with f' to high order, we need

$$a+b+c = 0$$

$$-b-2c = 1/h$$

$$\frac{b}{2} + 2c = 0$$

3 eqs, 3 unknowns

\Rightarrow

$$-2c = \frac{1}{h} \rightarrow c = -\frac{1}{2h}$$

$$\rightarrow b = -4c$$

$$\rightarrow a = -b-c = \frac{2}{h} - \frac{1}{2h} = \frac{3}{2h}$$

$$= \frac{3}{2h}$$

$$\downarrow b = -\frac{2}{h}$$

$$a = \frac{3}{2h}, b = -\frac{2}{h}, c = -\frac{1}{2h}$$

General Approach:

Suppose we want to approximate the k^{th} derivative of f using the value of f at x_1, \dots, x_n .

$$D_k f = c_1 f(x_1) + \dots + c_n f(x_n) = f^{(k)}(\bar{x}) + O(h^p)$$

(doesn't assume equal spacing!)

Expand about x :

$$f(x_i) = f(x) + f'(x)(x_i - x) + \frac{1}{2!} f''(x)(x_i - x)^2 + \dots + \frac{1}{k!} f^{(k)}(x)(x_i - x)^k + \dots + \frac{1}{(n-1)!} f^{(n-1)}(x)(x_i - x)^{n-1}$$

Group by derivative order:

$$D_k f = f(x) \sum_{i=1}^n c_i + f'(x) \sum_{i=1}^n c_i (x_i - x) + \dots + f^{(k)}(x) \sum_{i=1}^n \frac{1}{k!} c_i (x_i - x)^k + \dots$$

$$\Rightarrow \frac{1}{(i-k)!} \sum_{j=1}^n c_j (x_j - x)^{(i-k)} = \begin{cases} 1 & \text{if } i-k = k \\ 0 & \text{otherwise} \end{cases}$$

$$i = 1, 2, \dots, n$$

n unknowns, n equations

can be written

\Rightarrow

$$\underline{A} \underline{c} = \underline{b}$$

\uparrow
Vandermonde matrix. (non-singular, but ill-conditioned)

$$\underline{A} \in \mathbb{R}^{n \times n}, \underline{c} \in \mathbb{R}^n, \underline{b} \in \mathbb{R}^n$$

$$\underline{b} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \leftarrow (k+1)^{\text{th}} \text{ entry}$$

$$\Rightarrow \text{need } k+1 \leq n!$$

$$\text{otherwise, } \underline{b} = 0 \Rightarrow \underline{c} = 0!$$

Why care about 1-sided differences?

- time derivatives
- Neumann B.C.s
- stability (i.e. lin. advection)

ODE Solvers

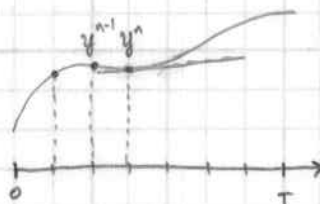
General system of ODEs (nonlinear in general)

$$\underline{M} \dot{y} = r(t, y), \quad \underline{M} \in \mathbb{R}^{n \times n}, \quad y \in \mathbb{R}^n, \quad t \in \mathbb{R}_+, \quad r: \mathbb{R}^n \times \mathbb{R}_+ \rightarrow \mathbb{R}^n$$

velocity = $\underline{M}^{-1} r(t, y)$

Types of ODE schemes:

- Implicit vs. Explicit vs. IMEX
- Single stage vs. multi-stage
- Single step vs. multi-step
- Serial vs. Parallel



Simplest explicit: forward Euler

$$\underline{M} y^{n+1} = \underline{M} y^n + \Delta t r(t_n, y^n)$$

$$\downarrow$$

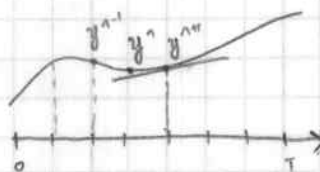
$$y^{n+1} = y^n + \Delta t \underline{M}^{-1} r(t_n, y^n)$$

usually \underline{M} diagonal or block diagonal (or approximated as so) $\Rightarrow \underline{M}^{-1}$ cheap!

Simplest implicit: backward Euler

$$\underline{M} y^{n+1} = \underline{M} y^n + \Delta t r(t_{n+1}, y^{n+1})$$

$$y^{n+1} = y^n + \Delta t \underline{M}^{-1} r(t_{n+1}, y^{n+1})$$



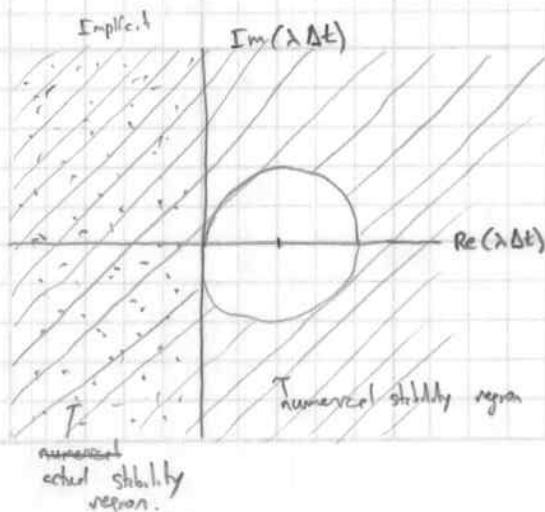
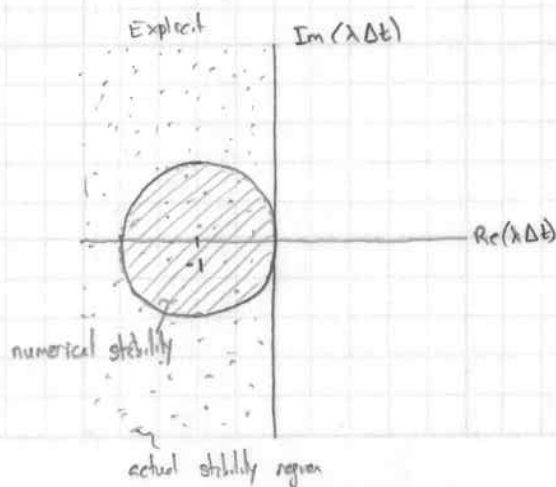
Analysis on simple model problem: $\dot{y} = \lambda y \rightarrow$ exact solution: $y = y(0) e^{\lambda t}$
 \hookrightarrow stable if $\text{Re } \lambda < 0$

explicit: $y^{n+1} = y^n + \lambda \Delta t y^n = (1 + \lambda \Delta t) y^n$

$\Rightarrow y^{n+1} = (1 + \lambda \Delta t)^{n+1} y^0 \rightarrow$ goes to infinity if $|1 + \lambda \Delta t| > 1$ (unstable)

implicit: $y^{n+1} = y^n + \lambda \Delta t y^{n+1}$

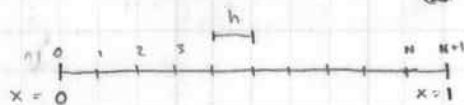
$\Rightarrow y^{n+1} = \frac{1}{1 - \lambda \Delta t} y^n = \frac{1}{(1 - \lambda \Delta t)^{n+1}} y^0 \rightarrow$ unstable if $\frac{1}{|1 - \lambda \Delta t|} > 1$



Truncation Error, Consistency, Convergence

Consider the PDE : $u''(x) = f(x)$ $0 < x < 1$
 $u(0) = \alpha, u(1) = \beta$

Finite Difference approximation :



$$\frac{1}{h^2}(\bar{u}_{j+1} - 2\bar{u}_j + \bar{u}_{j-1}) = f(x_j) \quad j=1, \dots, N$$

$$\bar{u}_0 = \alpha, \bar{u}_{N+1} = \beta$$

Local truncation error :

\bar{u}_j = fin. d.f. approx. to $u(x_j)$

Replace u_j w/ exact solution $u(x_j)$:

$$\begin{aligned} \tau_j &= (u(x_{j+1}) - 2u(x_j) + u(x_{j-1})) \frac{1}{h^2} - f(x_j) \quad j=1, \dots, N. \\ &= u''(x_j) + \frac{h^2}{12} u'''(x_j) + O(h^4) - f(x_j) \quad \text{from (A) on pg. 1. (Taylor series).} \\ &= \frac{h^2}{12} u'''(x_j) + O(h^4) \quad \text{since } u''(x_j) - f(x_j) = 0. \end{aligned}$$

$$\tau_j = O(h^4) \Rightarrow h \rightarrow 0$$

Matrix notation : $AU = F$

$$A = \frac{1}{h^2} \begin{bmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \\ & & 1 & -2 \end{bmatrix} \quad U = \begin{bmatrix} \bar{u}_1 \\ \vdots \\ \bar{u}_N \end{bmatrix} \quad F = \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_N) \end{bmatrix} - \frac{1}{h^2} \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \\ \beta \end{bmatrix}$$

Global error : Subtract (20) from (18) [fin. d.f. eqn. from local trunc. eqn] :

$$\tau = \begin{bmatrix} \tau_1 \\ \vdots \\ \tau_N \end{bmatrix}$$

and define $e_j = \bar{u}_j - u(x_j)$. [clearly $e_0 = e_N = 0$]

$$\frac{1}{h^2}(e_{j+1} - 2e_j + e_{j-1}) = -\tau_j \quad j=1, \dots, N$$

$$AE = -\tau$$

$$E = U - U_{\text{exact}}$$

$$e_0 = e_N = 0.$$

\Rightarrow error satisfies finite difference equation nearly identical to original equation :

interpret as discretization of :

$$e''(x) = -\tau(x) \quad x \in (0, 1)$$

$$e(0) = e(1) = 0.$$

Since $\tau(x) \approx \frac{h^2}{12} u'''(x)$, integration shows that:

$$e(x) \approx -\frac{1}{12} h^2 u'''(x) + \frac{1}{12} h^2 (u'''(0) + x(u'''(1) - u'''(0)))$$

$$\Rightarrow \boxed{e(x) = O(h^2)} \quad \square$$

$$\frac{\partial \phi}{\partial t} + \frac{\partial^3 \phi}{\partial x^3} + 6\phi \frac{\partial \phi}{\partial x} = 0 \Rightarrow \frac{\partial \phi}{\partial t} + D_3 \phi + 6(\text{diag } \phi)(D_1 \phi) = 0.$$

explicit: $\phi^{n+1} = \phi^n - \Delta t [D_3 \phi^n + 6(\text{diag } \phi^n)(D_1 \phi^n)]$

implicit: $\phi^{n+1} = \phi^n - \Delta t [D_3 \phi^{n+1} + 6(\text{diag } \phi^{n+1})(D_1 \phi^{n+1})]$

↑

need derivatives for
implicit b/c you
must apply Newton's
method to solve the
equation $R(\phi) = 0$:

$$\phi_{k+1}^{n+1} = \phi_k^{n+1} - \frac{\partial R}{\partial \phi}(\phi_k^{n+1})^{-1} R(\phi_k^{n+1})$$

$$\frac{\partial}{\partial \phi_{j-1}} [\phi_j (\phi_{j+1} - \phi_{j-1}) \frac{1}{2h}] = \phi_j (-1) \frac{1}{2h}$$

$$\frac{\partial}{\partial \phi_{j+1}} [\phi_j (\phi_{j+1} - \phi_{j-1}) \frac{1}{2h}] = \phi_j (1) \frac{1}{2h}$$

$$\frac{\partial}{\partial \phi_j} [\cdot] = (\phi_{j+1} - \phi_{j-1}) \frac{1}{2h}$$

$$[\phi_j (-\phi_{j-1}) \frac{1}{2h}, (\phi_{j+1} - \phi_{j-1}) \frac{1}{2h}, \phi_j (\phi_{j+1}) \frac{1}{2h}]$$

$$= D_1 \phi + \text{diag } \phi \cdot D_1$$