Equations with non-constant coefficients

Diffusion equation

Let $u(x,t)$ is defined for $x \in [0,1]$ and $t \in [0,T]$.

$$q(x,t)\,\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(p(x,t)\frac{\partial u}{\partial x}\right) + f(x,t) \tag{1}$$

Note $q(x,t)$ and $p(x,t)$.

Initial condition:

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

Boundary conditions

$$u(0,t) = \mu_1(t) \qquad\qquad u(1,t) = \mu_2(t)$$

The Sturm-Liouville operator

Need to approximate the Sturm-Liouville operator

$$Lu = \frac{\partial}{\partial x}\left(p(x,t)\frac{\partial u}{\partial x}\right)$$

Use at (x_j, t)

$$\Lambda(t)y_j = \frac{1}{h}\left(a_{j+1}(t)\,\frac{y_{j+1} - y_j}{h} - a_j(t)\,\frac{y_j - y_{j-1}}{h}\right)$$

The Sturm-Liouville operator

The FD diffusivity, a_j, needs to satisfy the *second order approximation conditions*

$$\frac{a_{j+1}(t) + a_j(t)}{2} = p(x_j, t) + O(h^2)$$

$$\frac{a_{j+1}(t) - a_j(t)}{h} = p'(x_j, t) + O(h^2)$$

For example,

$$a_j(t) = p(x_j - h/2, t)\,, \quad \text{or}$$
$$a_j(t) = (p(x_j, t) + p(x_{j-1}, t))/2\,,$$
$$\text{etc}$$

Approximation of the PDE

Now approximate the r.h.s. of the PDE (1) using a scheme with weights on the six-point stencil

$$u(x_j, t_n) \longrightarrow \sigma y_j^{n+1} + (1-\sigma) y_j^n$$

Then

$$q(x_j, t)\, \frac{y_j^{n+1} - y_j^n}{\tau} = \Lambda(t) \left[\sigma y_j^{n+1} + (1-\sigma) y_j^n \right] + f(x_j, t)$$

with $t \in [t_n, t_{n+1}]$

Approximation of the PDE

The scheme

$$q(x_j,t)\,\frac{y_j^{n+1}-y_j^n}{\tau} = \Lambda(t)\left[\sigma y_j^{n+1} + (1-\sigma)y_j^n\right] + f(x_j,t)$$

approximates the PDE (1) with

- $O(\tau^2+h^2)$ if $t = t_n + \tau/2$ and $\sigma = 1/2$
- $O(\tau+h^2)$ otherwise

Stability: the method of frozen coefficients

- Pretend that the coefficients are constant.
- Analyze the von Neumann stability.
- Require that the scheme is stable for all allowed values of $p(x,t)$ and $q(x,t)$

This guarantees stability of the scheme iff the coefficients are smooth enough.

The method of frozen coefficients

As an example, consider the explicit scheme with $\sigma = 0$ for $f(x,t) = 0$

$$q(x_j, t)\,\frac{y_j^{n+1} - y_j^n}{\tau} = \Lambda(t) y_j^n$$

Pretend that

$$q(x,t) = q = \text{const}\,, \qquad \text{and} \qquad a(x,t) = a = \text{const}$$

The FD scheme becomes $$q\,\frac{y_j^{n+1} - y_j^n}{\tau} = a\,\mathcal{D}_{xx} y_j^n$$

The method of frozen coefficients

Absorb the coefficients into the step size:

$$\frac{y_j^{n+1} - y_j^n}{\tau_1} = \mathcal{D}_{xx} y_j^n$$

with $\tau_1 = \tau a/q$.

Which is stable for $\tau_1 \leqslant h^2/2$

Then, the original scheme is von Neumann stable if

$$\frac{a(x,t)}{q(x,t)}\tau \leqslant \frac{h^2}{2} \qquad\qquad \forall x, t \in \Omega$$

Nonlinear equations

Nonlinear parabolic equation

Let $u(x,t)$ is defined for $x \in [0,1]$ and $t \in [0,T]$.

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(p(u)\frac{\partial u}{\partial x}\right) + f(u) \tag{2}$$

Initial condition:

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

Boundary conditions

$$u(0,t) = \mu_1(t) \qquad\qquad u(1,t) = \mu_2(t)$$

Nonlinear parabolic equation

Typically, avoid explicit schemes for non-linear equations.

Construct a scheme which is

- Implicit w.r.t. y^{n+1}
- Linear w.r.t. y^{n+1}

An implicit linear scheme

$$\frac{y_j^{n+1} - y_j^n}{\tau} = \frac{1}{h}\left[a_j^n \, \frac{y_{j+1}^{n+1} - y_j^{n+1}}{h} - a_j^n \, \frac{y_j^{n+1} - y_{j-1}^{n+1}}{h}\right] + f(y_j^n)$$

with

$$a_j^n = \frac{1}{2}\big(p(y_j^n) + p(y_{j-1}^n)\big)$$

- Note that the nonlinearities are at y^n
- Solve for y^{n+1} via a tridiagonal solve
- The scheme is unconditionally stable
- The scheme approximates Eq. (2) with $O(\tau + h^2)$

A nonlinear scheme

Evaluate non-linear terms at y^{n+1}:

$$\frac{y_j^{n+1} - y_j^n}{\tau} = \frac{1}{h}\left[a_j^{n+1}\,\frac{y_{j+1}^{n+1} - y_j^{n+1}}{h} - a_j^{n+1}\,\frac{y_j^{n+1} - y_{j-1}^{n+1}}{h}\right] + f(y_j^{n+1})$$

with

$$a_j^{n+1} = \frac{1}{2}\big(p(y_j^{n+1}) + p(y_{j-1}^{n+1})\big)$$

At each layer, need to solve *nonlinear* equations for y^{n+1}.

A nonlinear scheme

Transition $n \longrightarrow n+1$: solve nonlinear equations for y^{n+1}.

Use an iterative method: construct a sequence of $M = \mathrm{const}$ steps:

$$y_j^{(s)}\,, \qquad j = 1, \cdots, N\,, \qquad\qquad s = 0, 1, \cdots, M$$

with

$$y_j^{(0)} = y_j^n\,, \qquad \text{and} \qquad y_j^{(M)} = y_j^{n+1}$$

NB: use a fixed number, M, of *inner* iterations.

A nonlinear scheme

Label inner iterations by s:

$$\frac{y_j^{(s+1)} - y_j^n}{\tau} = \frac{1}{h}\left[a_j^{(s)}\,\frac{y_{j+1}^{(s+1)} - y_j^{(s+1)}}{h} - a_j^{(s)}\,\frac{y_j^{(s+1)} - y_{j-1}^{(s+1)}}{h}\right] + f(y_j^{(s)})$$

with $s = 0, 1, \cdots, M-1$, $\quad y_j^{(0)} = y_j^n$ and $y_j^{(M)} = y_j^{n+1}$

- $M = 1$ is a linear scheme.
- The nonlinear coefficients are evaluated at the "previous iteration", s
- Solving for y^{s+1} is a tridiagonal solve.

A predictor-corrector type scheme

Transition $n \longrightarrow n+1$ via an auxilliary layer $n+1/2$.

Step 1: $n \longrightarrow n+1/2$

Use an implicit linear scheme

$$\frac{w_j - y_j^n}{\tau/2} = \frac{1}{h}\left[a_j^n \, \frac{w_{j+1} - w_j}{h} - a_j^n \, \frac{w_j - w_{j-1}}{h}\right] + f(y_j^n)$$

$$w_0 = \mu_1(t_n + \tau/2)\,, \qquad w_N = \mu_2(t_n + \tau/2)$$

Here $w_j \equiv y_j^{n+1/2}$

NB: nonlinear coefficients are at layer n.

A predictor-corrector type scheme

Transition $n \longrightarrow n+1$ via an auxilliary layer $n+1/2$.

Step 2: $n \longrightarrow n+1$

Use the Crank-Nicholson scheme with nonlinear coefficients evaluated at $y^{n+1/2}$:

$$\frac{y_j^{n+1} - y_j^n}{\tau} = \frac{1}{2}\left[\mathcal{D}_x\left(a_j \mathcal{D}_x y_j^{n+1}\right) + \mathcal{D}_x\left(a_j \mathcal{D}_x y_j^n\right)\right] + f_j$$

Here $f_j \equiv f(y_j^{n+1/2})$ and $a_j \equiv a(y_j^{n+1/2})$