Diffusion Equation

Method of Lines. (MOL)

- Brodie refers to this as semi-discretization.

- Basic Idea: $u_t = \alpha^2 u_{xx}$ $\quad t \geq 0 \quad 0 \leq x \leq 1$

$u(0,t) = \varphi_0(t)$ $\qquad u(x,0) = g(x)$

$u(1,t) = \varphi_1(t)$

Discretize in space only.

$$\Rightarrow \frac{\partial}{\partial t} u(x_n,t) = \alpha^2 \frac{u(x_{n-1},t) - 2u(x_n,t) + u(x_{n+1},t)}{h^2} + \mathcal{O}(h^2)$$

In vector form

$$\frac{\partial}{\partial t}\begin{bmatrix} u_1(t) \\ u_2(t) \\ \vdots \\ \vdots \\ u_n(t) \end{bmatrix} = \frac{\alpha^2}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & -2 \end{bmatrix} \underbrace{\begin{bmatrix} u_1(t) \\ u_2(t) \\ \vdots \\ \vdots \\ u_n(t) \end{bmatrix}}_{\underline{u}(t)} + \frac{\alpha^2}{h^2}\begin{bmatrix} \varphi_0(t) \\ 0 \\ \vdots \\ \vdots \\ \varphi_1(t) \end{bmatrix} + \mathcal{O}(h^2)$$

$$\Rightarrow \boxed{\frac{\partial}{\partial t} u(x,t) \approx \frac{d}{dt}\underline{u}(t) = \alpha^2 D_{2,x}\, \underline{u}(t) + \frac{\alpha^2}{h^2}\varphi_0(t) e_1 + \frac{\alpha^2}{h^2}\varphi_1(t) e_n}$$

$\Rightarrow$ we have semi-discretized the PDE so that it is now a coupled linear system of ODEs.

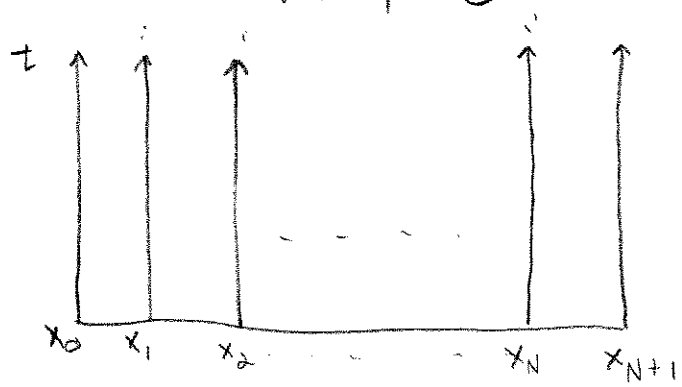
Diffusion Equation.

- Origin of MOL

- Together with the initial conditions

$$U_1(0)=g(x_1),\quad U_2(0)=g(x_2),\quad \dots\quad, U_N(0)=g(x_n),$$

the approximate solution of the PDE is given by the solution of the system of ODEs on lines in the (x,t) plane



- Coupling the semi-discretization with ODE solver

- Now that we have reduced the problem to a linear system of ODEs, we can try to apply any of the ODE methods we learned to advance the system forward in time.

General ODE method: Problem

$$u'(t) = f(t,\underline{u}) \qquad t\geq 0 \quad \underline{u}(0)=\underline{g}.$$

Our problem is with

$$f(t,\underline{u}) = D_{2x}\underline{u}(t) + \frac{\alpha^2}{h^2}\varphi_0(t)\underline{e}_1 + \frac{\alpha^2}{h^2}\varphi_1(t)\underline{e}_N$$

- We can now apply our knowledge for ODE methods (e.g. stability, adaptivity, error control) to PDE methods

Diffusion Equation

Forward Euler:

$$\underline{u}^{j+1} = \underline{u}^{j} + k\,\underline{f}^{j}$$

$$\Rightarrow \underbrace{\underline{u}^{j+1} = \underline{u}^{j} + \alpha^2 k D_{2x}\underline{u}^{j} + \frac{\alpha^2}{h^2}\varphi_0(t_j)e_1 + \frac{\alpha^2}{h^2}\varphi_1(t_j)e_N}_{\text{Same as Full discretization scheme}}$$

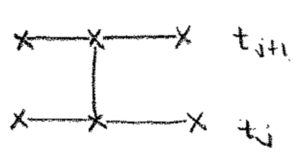
- Similar for backward Euler.

- Trapezoidal Rule (AM2)

$$\underline{u}^{j+1} = \underline{u}^{j} + \frac{\alpha^2 k}{2}\left[D_2\underline{u}^{j+1} + D_2\underline{u}^{j}\right] + \frac{\alpha^2}{2h^2}\Big[\big(\varphi_0(t_{j+1}) + \varphi_0(t_j)\big)e_1 + \big(\varphi_1(t_{j+1}) + \varphi_1(t_j)\big)e_N\Big]$$

$$\Rightarrow \boxed{\left(I - \frac{\alpha k}{2}D_{2x}\right)\underline{u}^{j+1} = \left(I + \frac{\alpha k}{2}D_{2x}\right)\underline{u}^{j} + (\text{Boundary Data})}$$

Stencil:



- Called $\boxed{\text{Crank-Nicholson}}$ when applied to PDEs.

- One of the most popular methods for solving the diffusion equation.

- Second order accurate in space and time and unconditionally stable.

Diffusion Equation

Example: $u_t = u_{xx}$ $(\alpha = 1)$ $0 \le x \le 1$ $t \ge 0$

$g(x) = \sin(\frac{\pi}{2}x) + \frac{1}{2}\sin(2\pi x)$

$\varphi_0(t) \equiv 0$, $\varphi_1(t) = e^{-\pi^2 t/4}$

Max Error: $u(1,x)$

	k = 1/128	1/256	1/512
1/8	7.53×10^{-5}	7.59×10^{-5}	7.60×10^{-5}
1/16	1.84×10^{-5}	1.89×10^{-5}	1.91×10^{-5}
1/32	4.04×10^{-6}	4.59×10^{-6}	4.73×10^{-6}

Reduced by a factor of 4

Convergence

- Recall that a numerical method is useless unless it converges to the true solution.

- Like the Dahlquist equivalence theorem, the following theorem gives us an algebraic set of conditions to determine convergence

- The theorem works for general linear evolutionary PDES

$$\frac{\partial}{\partial t} u(\underline{x},t) = \mathcal{L} u(\underline{x},t) + f \qquad t \ge 0$$

$\mathcal{L}$ is some linear differential operator

i.e. $\mathcal{L} = \nabla^2, \frac{\partial^2}{\partial x^2}, \frac{\partial}{\partial x}, \nabla,$ etc.

- We will apply it to $u_t = \alpha^2 u_{xx}$ & $u_t + c u_x = 0$