The Heat/Diffusion Equation

The heat (or diffusion) equation is \((D > 0)\)

\[
\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}, \quad u(x, t = 0) = u_0(x).
\]

The fundamental solution or kernel \(K(x,t)\) of the heat/diffusion equation is

\[
K(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left\{ -\frac{x^2}{4Dt} \right\}
\]

which satisfies the initial value problem

\[
\frac{\partial K}{\partial t} = D \frac{\partial^2 K}{\partial x^2}, \quad K(x, t = 0) = \delta(x).
\]

Note that \(\int_{-\infty}^{\infty} K(x,t) \, dx = 1\) for any \(t\).

The general solution to the heat/diffusion equation is

\[
u(x,t) = \int_{-\infty}^{\infty} K(x - y, t) \, u_0(y) \, dy = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} \exp\left\{ -\frac{(x - y)^2}{4Dt} \right\} \, u_0(y) \, dy.
\]
$K(x-y, t)$ is also the Green’s function $G(x, y; t)$ for the homogeneous heat/diffusion equation.

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Table 1: Numerical methods for the heat/diffusion equation $u_t = Du_{xx}$.

The **backward Euler** numerical method

$\frac{u_i^{n+1} - u_i^n}{\Delta t} = D \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2}$

$u_i^{n+1} = u_i^n + D \frac{\Delta t}{\Delta x^2} \left( u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1} \right)$

is first-order accurate and A-stable and L-stable.

**Consistency:** The LTE $= \Delta t \tau$ is given by

$u(t+\Delta t) = u + \frac{D\Delta t}{h^2} (u(x+h, t+\Delta t) - 2u(x, t+\Delta t) + u(x-h, t+\Delta t)) + \Delta t \tau.$

Taylor expanding, we get

$u + \Delta t u_t + \frac{\Delta t^2}{2} u_{tt} + \cdots = u + D\Delta t \left( u_{xx} + \Delta t u_{xxt} + \frac{h^2}{12} u_{xxxx} + \cdots \right) + \Delta t \tau$

$\tau = -\frac{\Delta t}{2} u_{tt} - \frac{Dh^2}{12} u_{xxxx} + \cdots$

**Stability:** To analyze stability, we will use von Neumann’s Fourier analysis method. General initial data at time $t$ can be represented by a Fourier integral

$u(x, t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} u_k(t)$

where $e^{ikx} = \cos(kx) + i \sin(kx)$. Then after a timestep of $\Delta t$,

$u(x, t + \Delta t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} G(k) u_k(t).$
Now set \( u^n_j \) equal to a single Fourier mode \( u^n_j = e^{ikx_j} \), and derive the growth factor \( u^{n+1}_j = G(k)u^n_j \) for this mode. Then we require that \( |G(k)| \leq 1 \) for all \( k \). We find

\[
0 < G(k) = \frac{1}{1 + \frac{4D\Delta t}{h^2} \sin^2 \left( \frac{kh}{2} \right)} \leq 1
\]

so backward Euler is A-stable. Backward Euler is L-stable as well, since \( \lim_{\Delta t \to \infty} |G| = 0 \).

**Derivation of \( G(k) \).** Set \( u^n_j = e^{ikx_j} \) and \( u^{n+1}_j = G(k)u^n_j = G(k)e^{ikx_j} \) in the backward Euler method:

\[
u^{n+1}_j = Ge^{ikx_j} = u^n_j + \frac{D\Delta t}{h^2} \left( u^{n+1}_{j+1} - 2u^{n+1}_j + u^{n+1}_{j-1} \right) =
\]

\[
e^{ikx_j} + \frac{D\Delta t}{h^2} G \left( e^{ikx_{j+1}} - 2e^{ikx_j} + e^{ikx_{j-1}} \right) =
\]

\[
e^{ikx_j} + \frac{D\Delta t}{h^2} \left( e^{ikh} - 2 + e^{-ikh} \right) Ge^{ikx_j} =
\]

\[
e^{ikx_j} + \frac{2D\Delta t}{h^2} \left( \cos(kh) - 1 \right) Ge^{ikx_j} =
\]

\[
e^{ikx_j} - \frac{4D\Delta t}{h^2} \sin^2 \left( \frac{kh}{2} \right) Ge^{ikx_j}.
\]

Now solving for \( G \) yields

\[
G = 1 - \frac{4D\Delta t}{h^2} \sin^2 \left( \frac{kh}{2} \right) G
\]

\[
G(k) = \frac{1}{1 + \frac{4D\Delta t}{h^2} \sin^2 \left( \frac{kh}{2} \right)}.
\]

**Relationship to ODEs.** Parabolic PDEs are closely related to stiff ODEs. In fact, if the heat/diffusion equation \( u_t = Du_{xx} \) is discretized in space using three-point central differences, the errors \( \tau \) and growth factors \( G(k) \) for the original PDE are related to those for the ODE \( du/dt = -\alpha u, \alpha > 0 \), for forward Euler, backward Euler, TR, TRBDF2, etc. by the transcription:

\[
\tau = \tau_{ODE} - \frac{h^2 D}{12} u_{xxxx} + \cdots
\]
\[ G(k) = G_{ODE}(\alpha \Delta t), \quad \alpha = \frac{4D}{h^2} \sin^2 \left( \frac{kh}{2} \right). \]

**Fourier Solution.** The Fourier solution to the initial/boundary value problem for the heat/diffusion equation with homogeneous Dirichlet boundary conditions

\[ u_t = u_{xx}, \quad u(0, t) = 0 = u(\pi, t), \quad u(x, t = 0) = u_0(x) \]

is obtained by making a Fourier sine expansion (since it automatically satisfies the boundary conditions)

\[ u(x, t) = \sum_{n=1}^{\infty} a_n(t) \sin(nx) \]

where

\[ a_n(0) = \frac{2}{\pi} \int_0^{\pi} \sin(nx) u_0(x) \, dx. \]

Plugging the Fourier expansion into the heat/diffusion equation and using orthogonality of the sines, we have

\[ \sum_{n=1}^{\infty} \frac{da_n}{dt} \sin(nx) = -\sum_{n=1}^{\infty} n^2 a_n \sin(nx) \]

\[ \frac{da_n}{dt} = -n^2 a_n, \quad a_n(t) = a_n(0)e^{-n^2 t} \]

and therefore

\[ u(x, t) = \sum_{n=1}^{\infty} a_n(0)e^{-n^2 t} \sin(nx). \]

This is an example of a spectral method solution. On the computer, \( u(x, t) \) is approximated by

\[ u_N(x, t) = \sum_{n=1}^{N} a_n(t) \sin(nx) \]

and the error

\[ ||u(x, t) - u_N(x, t)|| \sim e^{-N^2 t} \rightarrow 0 \]

as \( N \rightarrow \infty \) faster than any finite power of \( 1/N \) (so called “infinite” order accuracy).
Orthogonality relations. For the Fourier sine and cosine series solutions, we make use of the orthogonality relations ($m$ and $n$ are positive (non-negative) integers for sin (cos))

\[ \int_0^\pi \sin(mx) \sin(nx) \, dx = \frac{\pi}{2} \delta_{mn} \]

\[ \int_0^\pi \sin(mx) \cos(nx) \, dx = 0 \]

\[ \int_0^\pi \cos(mx) \cos(nx) \, dx = \frac{\pi c_n}{2} \delta_{mn} \]

where $c_0 = 2$ and $c_n = 1$, $n \geq 1$. 