Numerical Methods for PDEs
Homework 1

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Problem 1

Suppose a double precision floating point number is stored on a computer using 64 bits in the following way: sign 1 bit, exponent 8 bits, and mantissa 55 bits. A given real number r is written as

$$r = \pm m 2^n$$

where the mantissa m satisfies $1/2 \leq m < 1$ and $-128 \leq n \leq 127$. Give the following numbers in both base 2 and base 10 scientific notation:

(a) What is the largest positive number *realmax* that can be stored?

(b) What is the smallest positive number *realmin* that can be stored?

(c) What is the machine epsilon ϵ_M (take the leading 1 in m to be a phantom)?

Solution: We calculate the largest positive number as

$$realmax \approx 2^{127} \approx 1.7014 \cdot 10^{38},$$

and the smallest positive number as

$$realmin = 2^{-128} \approx 1.4694 \cdot 10^{-39}.$$

Lastly, the machine epsilon is

$$\varepsilon_M = \frac{1}{2} 2^{-55} = 2^{-56} \approx 1.3878 \cdot 10^{-17}$$

Problem 2

(a) Verify that the three-point central difference formulas for df/dx and d^2f/dx^2 are second-order accurate.

Solution:
First lets verify for the three-point central difference formula for df/dx. Let $h = \Delta x$, then

$$\begin{aligned}
\left(\frac{df}{dx}\right)_i &\approx \frac{f_{i+1} - f_{i-1}}{2h} \\
&= \frac{\left(f_i + hf_1' + \frac{h^2}{2}f_i'' + \frac{h^3}{6}f_i''' + \cdots\right) - \left(f_i - hf_1' + \frac{h^2}{2}f_i'' - \frac{h^3}{6}f_i''' + \cdots\right)}{2h} \\
&= f_i' - \frac{h^2}{6}f_i''' + \cdots \\
&= f_i' + \mathcal{O}(h^2)\ .
\end{aligned}$$

Therefore, the three-point central difference for the first derivative in x is second-order accurate.
Now for d^2f/dx^2,

$$\begin{aligned}
\left(\frac{d^2f}{dx^2}\right)_i &\approx \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \\
&= \frac{\left(f_i + hf_1' + \frac{h^2}{2}f_i'' + \frac{h^3}{6}f_i''' + \frac{h^4}{24}f_i^{IV} + \cdots\right) - 2f_i + \left(f_i - hf_1' + \frac{h^2}{2}f_i'' - \frac{h^3}{6}f_i''' + \frac{h^4}{24}f_i^{IV} + \cdots\right)}{h^2} \\
&= f_i'' + \frac{h^2}{12}f_i^{IV} + \cdots \\
&= f_i'' + \mathcal{O}(h^2)\ .
\end{aligned}$$

Thus, the three-point central difference for the second derivative in x is second-order accurate.

(b) Verify that the one-sided difference formula

$$\frac{du}{dt} \approx \frac{u^{n+1} - u^n}{\Delta t}$$

is first-order accurate.

Solution:
We find that,

$$\begin{aligned}
\left(\frac{du}{dt}\right)^n &\approx \frac{u^{n+1} - u^n}{\Delta t} \\
&= \frac{\left(u^n + \Delta t\dot{u}^n + \frac{(\Delta t)^2}{2}\ddot{u}^n + \cdots\right) - u^n}{\Delta t} \\
&= \dot{u}^n + \frac{\Delta t}{2}\ddot{u}^n + \cdots \\
&= \dot{u}^n + \mathcal{O}(\Delta t)\ .
\end{aligned}$$

Thus, the one-sided difference formula is first-order accurate.

Problem 3

Verify that the approximation

$$\left(\frac{df}{dx}\right)_i = \frac{1}{\Delta x}\left[-\frac{1}{12}f_{i+2} + \frac{2}{3}f_{i+1} - \frac{2}{3}f_{i-1} + \frac{1}{12}f_{i-2}\right]$$

is fourth-order accurate.

Solution: We start by grouping the previous approximation,

$$\left(\frac{df}{dx}\right)_i = \frac{1}{3h}\left[\frac{1}{4}\left(f_{i-2} - f_{i+2}\right) + 2\left(f_{i+1} - f_{i-1}\right)\right],$$

and Taylor expanding the terms

$$f_{i\pm1} = f_i \pm hf_i' + \frac{h^2}{2}f_i'' \pm \frac{h^3}{6}f_i''' + \frac{h^4}{24}f_i^{IV} \pm \frac{h^5}{120}f_i^V + \ldots,$$

$$f_{i\pm2} = f_i \pm 2hf_i' + \frac{4h^2}{2}f_i'' \pm \frac{8h^3}{6}f_i''' + \frac{16h^4}{24}f_i^{IV} \pm \frac{32h^5}{120}f_i^V + \ldots$$

Further, it is easy to check that

$$\begin{aligned} f_{i-2} - f_{i+2} &= -4hf_i' - \frac{16h^3}{6}f_i''' - \frac{64h^5}{120}f_i^V + \ldots \\ &= -4hf_i' - \frac{8h^3}{3}f_i''' - \frac{8h^5}{15}f_i^V + \ldots, \end{aligned}$$

and

$$\begin{aligned} f_{i+1} - f_{i-1} &= 2hf_i' + \frac{2h^3}{6}f_i''' + \frac{2h^5}{120}f_i^V + \ldots \\ &= 2hf_i' + \frac{h^3}{3}f_i''' + \frac{h^5}{60}f_i^V + \ldots \end{aligned}$$

Finally, we just substitute in the approximation and obtain

$$\begin{aligned} \left(\frac{df}{dx}\right)_i &= \frac{1}{3h}\left[-hf_i' - \frac{2h^3}{3}f_i''' - \frac{2h^5}{15}f_i^V + 4hf_i' + \frac{2h^3}{3}f_i''' + \frac{2h^5}{60}f_i^V\right] \\ &= \frac{1}{3h}\left[3hf_i' - \frac{3h^5}{30}f_i^V\right] \\ &= f_i' - \frac{h^4}{30}f_i^V \\ &= f_i' + \mathcal{O}(h^4). \end{aligned}$$

Hence, the approximation is indeed fourth order accurate.

Problem 4

Show that the general solution to the heat equation

$$u(x,t) = \int_{-\infty}^{\infty} K(x-y,t)u_0(y)dy$$

where the fundamental solution or kernel

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

does in fact satisfy $u_t = \kappa\, u_{xx}$ with $u(x,t=0) = u_0(x)$. *Hint*: First show that K satisfies the heat equation. Then argue that u satisfies the heat equation. Finally show that u satisfies the initial conditions $u(x,t=0) = u_0(x)$.

Solution: First we calculate the time derivative of K,

$$K_t(x,t) = \frac{x^2}{4\kappa\sqrt{4\kappa\pi}} \frac{e^{\frac{-x^2}{4\kappa t}}}{t^{5/2}} - \frac{1}{2\sqrt{4\kappa\pi}} \frac{e^{\frac{-x^2}{4\kappa t}}}{t^{3/2}} \ .$$

Further we calculate the spatial derivatives,

$$K_x(x,t) = -\frac{2x}{4\kappa t\sqrt{4\kappa\pi t}} e^{\frac{-x^2}{4\kappa t}},$$

and

$$K_{xx}(x,t) = \frac{x^2}{4\kappa^2\sqrt{4\kappa\pi}} \frac{e^{\frac{-x^2}{4\kappa t}}}{t^{5/2}} - \frac{1}{2\kappa\sqrt{4\kappa\pi}} \frac{e^{\frac{-x^2}{4\kappa t}}}{t^{3/2}} \ .$$

Finally, it is easy to check that

$$\kappa K_{xx} = \frac{x^2}{4\kappa\sqrt{4\kappa\pi}} \frac{e^{\frac{-x^2}{4\kappa t}}}{t^{5/2}} - \frac{1}{2\sqrt{4\kappa\pi}} \frac{e^{\frac{-x^2}{4\kappa t}}}{t^{3/2}} = K_t(x,t),$$

and that K satisfies the heat equation. Now it is easier to check that u satisfies it as well,

$$\begin{aligned}
\kappa u_{xx} &= \kappa \frac{\partial^2}{\partial x^2} \int_{\infty}^{\infty} K(x-y,t)u_0(y)dy \\
&= \int_{\infty}^{\infty} \kappa K_{xx}(x-y,t)u_0(y)dy \\
&= \int_{\infty}^{\infty} K_t(x-y,t)u_0(y)dy \\
&= \frac{\partial}{\partial t} \int_{\infty}^{\infty} K(x-y,t)u_0(y)dy \\
&= \frac{\partial}{\partial t} u(x,t) \\
&= u_t.
\end{aligned}$$

To check that the initial condition is satisfied by this solution we take the limit,

$$\begin{aligned}
\lim_{t\to 0} u(x,t) &= \lim_{t\to 0}\int_{-\infty}^{\infty} K(x-y,t)u_0(y)dy \\
&= \int_{-\infty}^{\infty} \lim_{t\to 0} K(x-y,t)u_0(y)dy \\
&= \int_{-\infty}^{\infty} \delta(x-y)u_0(y)dy \\
&= u_0(x),
\end{aligned}$$

where we have used the fact that the limit at time zero of the heat kernel is the Dirac delta and its properties.

Problem 5

Show that the TR method for the heat equation $u_t = u_{xx}$

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

is second-order accurate, using the definition of the local truncation.

Solution:
Let $\Delta x = h$. We then substitute the true solution into the TR method and Taylor expand to find,

$$\begin{aligned}
u(x,t+\Delta t) = u(x,t) &+ \frac{\Delta t}{2}\left(u_{xx}(x,t) + \frac{h^2}{12}u_{xxxx}(x,t) + \cdots\right) \\
&+ \frac{\Delta t}{2}\left(u_{xx}(x,t+\Delta t) + \frac{h^2}{12}u_{xxxx}(x,t+\Delta t) + \cdots\right) + \Delta t\tau\ .
\end{aligned}$$

Letting $u(x,t) = u$ and Taylor expanding again, we find,

$$\begin{aligned}
u + \Delta t u_t + \frac{\Delta t}{2}u_{tt} + \cdots = u &+ \frac{\Delta t}{2}\left(u_{xx}(x,t) + \frac{h^2}{12}u_{xxxx}(x,t) + \cdots\right) \\
&+ \frac{\Delta t}{2}\left(u_{xx} + \Delta t u_{xxt} + \frac{\Delta t^2}{2}u_{xxtt} + \cdots\right) + \frac{\Delta t}{2}\left(u_{xxxx} + \Delta t u_{xxxxt} + \frac{\Delta t^2}{2}u_{xxxxtt} + \cdots\right) + \Delta t\tau\ .
\end{aligned}$$

Solving for τ, and noting the fact that $u_t = u_{xx}$, we get

$$\tau = \frac{-u_{xxtt}}{4}\Delta t^2 + \frac{-u_{xxxx}}{12}h^2 + \cdots\ .$$

Thus, the TR method for the heat equation is second-order accurate.