Numerical Methods for PDEs
Homework 3

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Problem 1

1. For the IVP $du/dt = f(u)$, derive the leading local error term (including the constant) for TRBDF2 using the definition of the LTE:
$$e_l \approx \text{LTE} \approx k_\gamma \Delta t^3 u''', \quad k_\gamma = \frac{-3\gamma^2 \ + \ 4\gamma \ - \ 2}{12(2-\gamma)}.$$
Hint: Set $u^{n+\gamma} = u(t_{n+\gamma}) - e_l^{TR}$. *Note:* For $u_t = Du_{xx}$,
$$\tau = k_\gamma \Delta t^2 u_{ttt} - \frac{h^2 D}{12} u_{xxxx} + \cdots$$

Solution: We start by substituting $u_{n+\gamma}$ in the *BDF2* step with the corresponding expression from the *TR* step, obtaining
$$u_{n+1} - \frac{1-\gamma}{2-\gamma}\Delta t_n f_{n+1} = \frac{1}{\gamma(2-\gamma)}\left[u_n + \gamma\frac{\Delta t_n}{2}\left(f_n + f_{n+\gamma}\right)\right] - \frac{(1-\gamma)^2}{\gamma(2-\gamma)}u_n. \tag{1}$$
Further, taking into account that $f_n = u_n'$, we Taylor expand the following terms:

- $f_{n+\gamma}$
$$f_{n+\gamma} = u_n' + \gamma\Delta t u_n'' + \gamma^2\frac{\Delta t^2}{2}u_n''' + \dots$$
- f_{n+1}
$$f_{n+1} = u_n' + \Delta t u_n'' + \frac{\Delta t^2}{2}u_n''' + \dots$$
- u_{n+1}
$$u_{n+1} = u_n + \Delta t u_n' + \frac{\Delta t^2}{2}u_n'' + \frac{\Delta t^3}{6}u_n''' + \dots$$

Introducing this terms into equation (1), and truncating the expansions after the third derivatives we obtain
$$\begin{aligned} u_n + \Delta t u_n' + \frac{\Delta t^2}{2}u_n'' + \frac{\Delta t^3}{6}u_n''' - \frac{1-\gamma}{2-\gamma}\Delta t_n\left(u_n' + \Delta t u_n'' + \frac{\Delta t^2}{2}u_n'''\right) \\ = \frac{1}{\gamma(2-\gamma)}\left[u_n + \gamma\frac{\Delta t_n}{2}\left(u_n' + u_n' + \gamma\Delta t u_n'' + \gamma^2\frac{\Delta t^2}{2}u_n'''\right)\right] - \frac{(1-\gamma)^2}{\gamma(2-\gamma)}u_n + e_l. \end{aligned}$$

Multiplying by $\gamma(2-\gamma)$ we get

$$u_n + \Delta t u_n' + \frac{\Delta t^2}{2} u_n'' + \frac{\Delta t^3}{6} u_n''' - \frac{1-\gamma}{2-\gamma} \Delta t_n \left(u_n' + \Delta t u_n'' + \frac{\Delta t^2}{2} u_n''' \right)$$
$$= \frac{1}{\gamma(2-\gamma)} \left[u_n + \gamma \frac{\Delta t_n}{2} \left(2u_n' + \gamma \Delta t u_n'' + \gamma^2 \frac{\Delta t^2}{2} u_n''' \right) \right] - \frac{(1-\gamma)^2}{\gamma(2-\gamma)} u_n + e_l.$$

Reorganizing terms:

$$\cancelto{0}{\left[1 - \frac{1}{\gamma(2-\gamma)} + \frac{(1-\gamma)^2}{\gamma(2-\gamma)}\right]} u_n + \cancelto{0}{\left[1 - \frac{1-\gamma}{2-\gamma} - \frac{1}{2-\gamma}\right]} \Delta t u_n'$$
$$+ \cancelto{0}{\left[1 - 2\frac{1-\gamma}{2-\gamma} - \frac{\gamma}{2-\gamma}\right]} \frac{\Delta t^2}{2} u_n'' + \left[1 - 3\frac{1-\gamma}{2-\gamma} - \frac{3}{2(2-\gamma)}\right] \frac{\Delta t^3}{6} u_n''' = e_l,$$

we finally get the desired result

$$e_l = \frac{-3\gamma^2 + 4\gamma - 2}{12(2-\gamma)} \Delta t^3 u_n'''$$

Problem 2

1. Derive the growth factor G for TRBDF2 for $du/dt = -\alpha u$, $\alpha > 0$, and show that the method is L-stable (assuming it is A-stable—proof given at the end of this problem set) for $0 < \gamma < 1$. *Hint:* First show that the growth factor is given by ($\Delta \equiv \gamma \alpha \Delta t > 0$):

$$G(\Delta t, \gamma) = \frac{\frac{1 - \frac{\gamma \alpha \Delta t}{2}}{1 + \frac{\gamma \alpha \Delta t}{2}} - (1-\gamma)^2}{\gamma(2-\gamma) + \gamma(1-\gamma)\alpha \Delta t} = \frac{\frac{2-\Delta}{2+\Delta} - (1-\gamma)^2}{\gamma(2-\gamma) + (1-\gamma)\Delta}.$$

Note: For $\gamma = 1$, the BDF2 step disappears, and $G \to G_{TR}$; similarly, for $\gamma = 0$, the TR step disappears, the BDF2 step $\to$ TR, and $G \to G_{TR}$. In both case, $k_\gamma \to -1/12$ (the TR value).

Also note that for $u_t = D u_{xx}$, $G(k)$ has the same form with

$$\alpha = \frac{4D}{h^2} \sin^2\left(\frac{kh}{2}\right).$$

Solution: We start by obtaining the growth function for the TR step. Let $u_{n+\gamma} = g^{TR}(k) u_n$ and, using the given PDE, $f_{n+\gamma} = -\alpha u_{n+\gamma} = -\alpha g^{TR}(k) u_n$. Hence,

$$u_{n+\gamma} - \gamma \frac{\Delta t_n}{2} f_{n+\gamma} = u_n + \gamma \frac{\Delta t_n}{2} f_n,$$
$$g^{TR}(k) u_n + \alpha \gamma \frac{\Delta t_n}{2} g^{TR}(k) u_n = u_n - \alpha \gamma \frac{\Delta t_n}{2} u_n,$$
$$g^{TR}(k) = \frac{1 - \alpha \gamma \frac{\Delta t_n}{2}}{1 + \alpha \gamma \frac{\Delta t_n}{2}},$$
$$g^{TR}(k) = \frac{2-\Delta}{2+\Delta},$$

where $\Delta = \alpha\gamma\Delta t$. We continue with the $BDF2$ step, noting that $u_{n+1} = g^{TR}(k)g^{BDF2}(k)u_n$ and $f_{n+1} = -\alpha u_{n+1} = -\alpha g^{TR}(k)g^{BDF2}(k)u_n$,

$$\begin{aligned}
u_{n+1} - \frac{1-\gamma}{2-\gamma}\Delta t f_{n+1} &= \frac{1}{\gamma(2-\gamma)}u_{n+\gamma} - \frac{(1-\gamma)^2}{\gamma(2-\gamma)}u_n \\
g^{TR}(k)g^{BDF2}(k)u_n + \alpha\frac{1-\gamma}{2-\gamma}\Delta t g^{TR}(k)g^{BDF2}(k)u_n &= \frac{1}{\gamma(2-\gamma)}g^{TR}(k)u_n - \frac{(1-\gamma)^2}{\gamma(2-\gamma)}u_n \\
g^{BDF2}(k) &= \frac{\frac{1}{\gamma(2-\gamma)}g^{TR}(k) - \frac{(1-\gamma)^2}{\gamma(2-\gamma)}}{g^{TR}(k) + \alpha\frac{1-\gamma}{2-\gamma}\Delta t g^{TR}(k)} \\
g^{BDF2}(k) &= \frac{g^{TR}(k) - (1-\gamma)^2}{\gamma(2-\gamma)g^{TR}(k) + \alpha\gamma(1-\gamma)\Delta t g^{TR}(k)}.
\end{aligned}$$

Finally,

$$G(k) = g^{TR}(k)g^{BDF2}(k) = \frac{g^{TR}(k) - (1-\gamma)^2}{\gamma(2-\gamma) + \alpha\gamma(1-\gamma)\Delta t},$$

$$G(k) = \frac{\frac{2-\Delta}{2+\Delta} - (1-\gamma)^2}{\gamma(2-\gamma) + (1-\gamma)\Delta}.$$

The method is L-stable since

$$\lim_{\Delta\to\infty} |G(k)| = \lim_{\Delta\to\infty} \left| \frac{\frac{2-\Delta}{2+\Delta} - (1-\gamma)^2}{\gamma(2-\gamma) + (1-\gamma)\Delta} \right| = 0,$$

since the denominator grows proportionally to Δ^2 and the numerator proportionally to Δ.

Problem 3

1. For $du/dt = f(u)$, derive

$$||e_l|| \equiv ||u(t_{n+1}) - u^{n+1}|| \approx \frac{3\gamma^2 - 4\gamma + 2}{3\gamma(1-\gamma)^2}\ ||u_1 - u_2||$$

for the TR/TR version of calculating the local error for TRBDF2, where $u_1 \equiv u^{n+1} = u_{TRBDF2}$ and $u_2 \equiv u_{TR/TR}$.

Solution: Equations (7) and (8) of the notes give us that

$$e_l = k_\gamma \Delta t_n^3 u''' \approx 2k_\gamma \Delta t_n \left(\frac{1}{\gamma} f_n - \frac{1}{\gamma(1-\gamma)} f_{n+\gamma} + \frac{1}{1-\gamma} f_{n+1} \right),$$

where

$$k_\gamma = \frac{-3\gamma^2 + 4\gamma - 2}{12(2-\gamma)}.$$

For the right hand side we first compute u_1, which is obtained by substituting $u_{n+\gamma}$ from the TR step into the $BDF2$ step (similar to what was done with equation (1) in the first problem),

$$u_1 = u_{n+1}^{TRBDF2} = \frac{1-\gamma}{2-\gamma}\Delta t_n f_{n+1} + \frac{1}{\gamma(2-\gamma)}\left[u_n + \gamma\frac{\Delta t_n}{2}\left(f_n + f_{n+\gamma}\right)\right] - \frac{(1-\gamma)^2}{\gamma(2-\gamma)}u_n.$$

Reorganizing and simplifying the previous equation,

$$u_1 = u_n + \frac{1}{2-\gamma}\frac{\Delta t_n}{2}f_n + \frac{1}{2-\gamma}\frac{\Delta t_n}{2}f_{n+\gamma} + \frac{1-\gamma}{2-\gamma}\Delta t_n f_{n+1}.$$

Further, we compute u_2 by taking to consecutives TR steps,

$$\begin{aligned} u_{n+\gamma} - \gamma\frac{\Delta t_n}{2}f_{n+\gamma} &= u_n + \gamma\frac{\Delta t_n}{2}f_n, \\ u_{n+1} - (1-\gamma)\frac{\Delta t_n}{2}f_{n+1} &= u_{n+\gamma} + (1-\gamma)\frac{\Delta t_n}{2}f_{n+\gamma}, \end{aligned}$$

obtaining

$$u_2 = u_{n+1}^{TR/TR} = (1-\gamma)\frac{\Delta t_n}{2}f_{n+1} + \gamma\frac{\Delta t_n}{2}f_{n+\gamma} + u_n + \gamma\frac{\Delta t_n}{2}f_n + (1-\gamma)\frac{\Delta t_n}{2}f_{n+\gamma},$$

$$u_2 = u_n + \gamma\frac{\Delta t_n}{2}f_n + \frac{\Delta t_n}{2}f_{n+\gamma} + (1-\gamma)\frac{\Delta t_n}{2}f_{n+1}.$$

Now we can compute the difference

$$u_1 - u_2 = \frac{(1-\gamma)^2}{2-\gamma}\frac{\Delta t_n}{2}f_n - \frac{1-\gamma}{2-\gamma}\frac{\Delta t_n}{2}f_{n+\gamma} + \gamma\frac{1-\gamma}{2-\gamma}\frac{\Delta t_n}{2}f_{n+1}$$

We can now prove the result

$$\begin{aligned} ||e_l|| &\approx \left|\left|2k_\gamma\Delta t_n\left(\frac{1}{\gamma}f_n - \frac{1}{\gamma(1-\gamma)}f_{n+\gamma} + \frac{1}{1-\gamma}f_{n+1}\right)\right|\right| \\ &= 2\Delta t_n|k_\gamma|\left|\left|\frac{1}{\gamma}f_n - \frac{1}{\gamma(1-\gamma)}f_{n+\gamma} + \frac{1}{1-\gamma}f_{n+1}\right|\right| \\ &= 2\Delta t_n\frac{3\gamma^2-4\gamma+2}{12(2-\gamma)}\left|\left|\frac{1}{\gamma}f_n - \frac{1}{\gamma(1-\gamma)}f_{n+\gamma} + \frac{1}{1-\gamma}f_{n+1}\right|\right| \\ &= \left|\left|2\Delta t_n\frac{3\gamma^2-4\gamma+2}{12(2-\gamma)}\left(\frac{1}{\gamma}f_n - \frac{1}{\gamma(1-\gamma)}f_{n+\gamma} + \frac{1}{1-\gamma}f_{n+1}\right)\right|\right| \\ &= \left|\left|\frac{3\gamma^2-4\gamma+2}{3\gamma(1-\gamma)^2}\left(\frac{(1-\gamma)^2}{2-\gamma}\frac{\Delta t_n}{2}f_n - \frac{1-\gamma}{2-\gamma}\frac{\Delta t_n}{2}f_{n+\gamma} + \gamma\frac{1-\gamma}{2-\gamma}\frac{\Delta t_n}{2}f_{n+1}\right)\right|\right| \\ &= \left|\left|\frac{3\gamma^2-4\gamma+2}{3\gamma(1-\gamma)^2}\left(u_1-u_2\right)\right|\right| \\ &= \frac{3\gamma^2-4\gamma+2}{3\gamma(1-\gamma)^2}\left|\left|u_1-u_2\right|\right|. \end{aligned}$$

Problem 4

1. Simulate nonlinear diffusion using TRBDF2.c. Plot (in one figure) $u(x,t)$ for $t = 0$, 500, 1000, 1500, 2000 sec ($t_{comp} = 0, 0.5, 1, 1.5, 2$) using the following parameters (for $t = 1000$ sec):

```
Enter the max value of t in 1000 sec: 1
Enter the max number of timesteps: 100000
Enter initial FACTOR & MAX_FACTOR for dt = FACTOR * dt_euler(t = 0): 10 100
Enter MIN_FACTOR for dt (e.g. 0.01): 0.01
Enter the min & max values of x in 0.1 microns: 0 10
Enter the number of dx: 100
```

Solution:

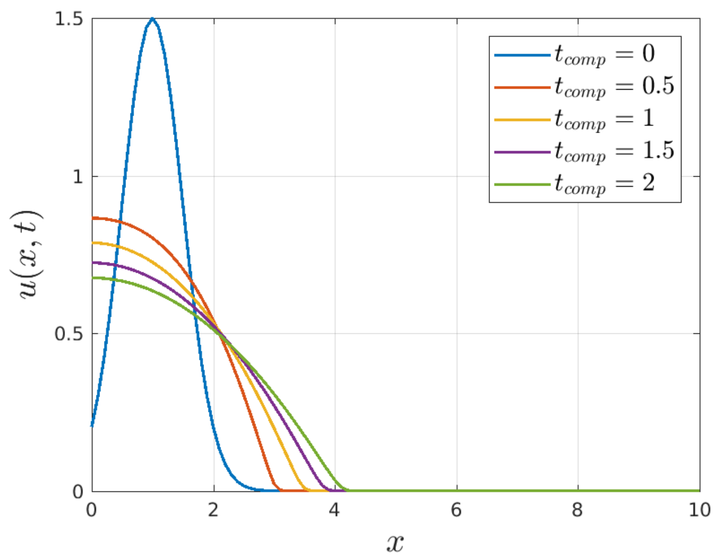

Figure 1: Funcion $u(x,t)$ for different values of time.

Problem 5

1. Verify that TRBDF2.c converges under mesh refinement. Plot $u(x,t)$ (in one figure) for $t = 500$ sec ($t_{comp} = 0.5$) for 25, 50, 100, and 200 Δx.

Solution:

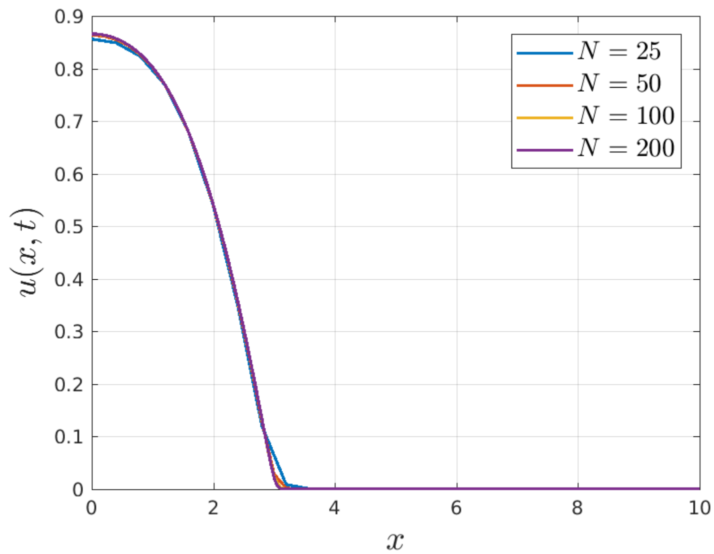

Figure 2: Solution $u(x, t = 500)$ for different mesh sizes.

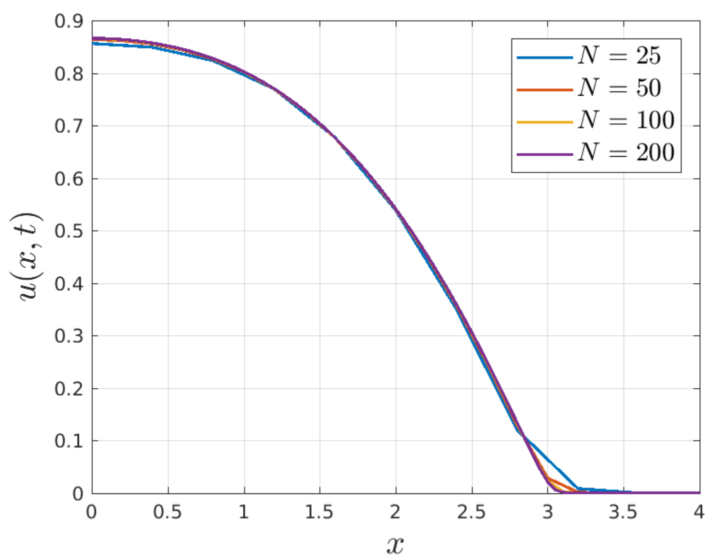

Figure 3: Zoom of figure (2).