Problem Set 3

Reading: LeVeque: Chapters 1, 9, E.1, E.2

Please label with APM 522, PS3, and your name; write up the problems neatly and succinctly (≤ 2 pages/problem, best if ≤ 1 page/problem) and in numerical order; and write (2) — if problem (2) is not attempted. No need to restate problem. Derive your answers!

(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:

\[
e_t \approx \text{LTE} \approx k_\gamma \Delta t^3 u''' \quad \text{where} \quad k_\gamma = \frac{-3\gamma^2 + 4\gamma - 2}{12(2 - \gamma)}.
\]

Hint: Set \( u^{n+\gamma} = u(t_{n+\gamma}) - e_t^{TR} \). Note: For \( u_t = D_{xx} \),

\[
\tau = k_\gamma \Delta t^2 u_{ttt} - \frac{h^2 D}{12} u_{xxxx} + \cdots
\]

(2) (5 pts) 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 \( (\Delta \equiv \gamma \alpha \Delta t > 0) \):

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

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

Also note that for \( u_t = D_{xx} \), \( G(k) \) has the same form with

\[
\alpha = \frac{4D}{h^2} \sin^2 \left( \frac{kh}{2} \right).
\]
(3) (5 pts) Verify the divided-difference estimate of the local error $e_l$:
\[ e_l = k \gamma \Delta t_n^2 u'' \approx 2k \gamma \Delta t_n \left( \frac{1}{\gamma} f_{n+\gamma} - \frac{1}{\gamma(1-\gamma)} f_{n+\gamma} + \frac{1}{1-\gamma} f_{n+1} \right). \]

(b) Show $|k \gamma|$ (and thus $||e_l||$) is minimized for $0 < \gamma = 2 - \sqrt{2} < 1$.

(4) For $du/dt = f(u)$, derive
\[ ||e_l|| \equiv ||u(t+1) - u^{n+1}|| \approx \frac{3\gamma^2 - 4\gamma + 2}{3(1-\gamma)^2} ||u_1 - u_2|| \]
for the TR/TR version of calculating the local error for TRBDF2, where $u_1 \equiv u^{n+1} = u_{TRBDF2}$ and $u_2 \equiv u_{TR/TR}$.

Please email me the two plots for (5) and (6) in PDF, png, jpeg, or eps — NOT a *.fig file!

(5) 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

(6) 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 $\Delta x$.

\[ (\star) \quad 1 \leq G = \frac{\frac{2-\Delta}{2+\Delta} - \theta_1^2}{\theta_2 + \theta_1 \Delta} \leq 1 \]
where $\Delta \equiv \gamma \alpha \Delta t > 0$ and
\[ 0 < \theta_1 = 1 - \gamma < 1, \quad 0 < \theta_2 = \gamma(2 - \gamma) < 1, \]
Note that
\[ \theta_1^2 + \theta_2 = 1, \quad \theta_1 + \theta_2 - 1 = \gamma(1 - \gamma) > 0 \]

Eq. (⋆) is equivalent to
\[ (⋆⋆) \quad - \theta_2 - \theta_1 \Delta + \theta_1^2 \leq \frac{2 - \Delta}{2 + \Delta} \leq \theta_2 + \theta_1 \Delta + \theta_1^2 = 1 + \theta_1 \Delta \]

and the right-hand inequality is true because \((2 - \Delta)/(2 + \Delta) \leq 1\), proving (i) \(G \leq 1\). From Eq. (⋆⋆), (ii) \(-1 \leq G \) iff
\[ 0 \leq 2 - \Delta + (2 + \Delta)(-\theta_1^2 + \theta_2 + \theta_1 \Delta) \]
iff
\[ 0 \leq 2 - \Delta + (2 + \Delta)(-1 + 2\theta_2 + \theta_1 \Delta) \]
iff
\[ 0 \leq \theta_1 \Delta^2 + 2(\theta_1 + \theta_2 - 1)\Delta + 4\theta_2 \]
which is manifestly true.