## Exercises from

## Finite Difference Methods for Ordinary and Partial Differential Equations

# by Randall J. LeVeque SIAM, Philadelphia, 2007

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## Chapter 1 Exercises

From: Finite Difference Methods for Ordinary and Partial Differential Equations by R. J. LeVeque, SIAM, 2007. http://www.amath.washington.edu/~rjl/fdmbook

#### Exercise 1.1 (derivation of finite difference formula)

Determine the interpolating polynomial p(x) discussed in Example 1.3 and verify that evaluation  $p'(\bar{x})$  gives equation (1.11).

#### Exercise 1.2 (use of fdstencil)

(a) Use the method of undetermined coefficients to set up the  $5 \times 5$  Vandermonde system that would determine a fourth-order accurate finite difference approximation to u''(x) based on 5 equally spaced points,

$$u''(x) = c_{-2}u(x-2h) + c_{-1}u(x-h) + c_0u(x) + c_1u(x+h) + c_2u(x+2h) + O(h^4).$$

- (b) Compute the coefficients using the MATLAB code fdstencil.m available from the website, and check that they satisfy the system you determined in part (a).
- (c) Test this finite difference formula to approximate u''(1) for  $u(x) = \sin(2x)$  with values of h from the array hvals = logspace(-1, -4, 13). Make a table of the error vs. h for several values of h and compare against the predicted error from the leading term of the expression printed by fdstencil. You may want to look at the m-file chap1example1.m for guidance on how to make such a table.

Also produce a log-log plot of the absolute value of the error vs. h.

You should observe the predicted accuracy for larger values of h. For smaller values, numerical cancellation in computing the linear combination of u values impacts the accuracy observed.

## Chapter 2 Exercises

From: Finite Difference Methods for Ordinary and Partial Differential Equations by R. J. LeVeque, SIAM, 2007. http://www.amath.washington.edu/~rjl/fdmbook

#### Exercise 2.1 (inverse matrix and Green's functions)

- (a) Write out the  $5 \times 5$  matrix A from (2.43) for the boundary value problem u''(x) = f(x) with u(0) = u(1) = 0 for h = 0.25.
- (b) Write out the  $5 \times 5$  inverse matrix  $A^{-1}$  explicitly for this problem.
- (c) If f(x) = x, determine the discrete approximation to the solution of the boundary value problem on this grid and sketch this solution and the five Green's functions whose sum gives this solution.

#### Exercise 2.2 (Green's function with Neumann boundary conditions)

(a) Determine the Green's functions for the two-point boundary value problem u''(x) = f(x) on 0 < x < 1 with a Neumann boundary condition at x = 0 and a Dirichlet condition at x = 1, i.e, find the function  $G(x, \bar{x})$  solving

$$u''(x) = \delta(x - \bar{x}), \quad u'(0) = 0, \quad u(1) = 0$$

and the functions  $G_0(x)$  solving

$$u''(x) = 0$$
,  $u'(0) = 1$ ,  $u(1) = 0$ 

and  $G_1(x)$  solving

$$u''(x) = 0$$
,  $u'(0) = 0$ ,  $u(1) = 1$ .

(b) Using this as guidance, find the general formulas for the elements of the inverse of the matrix in equation (2.54). Write out the  $5 \times 5$  matrices A and  $A^{-1}$  for the case h = 0.25.

#### Exercise 2.3 (solvability condition for Neumann problem)

Determine the null space of the matrix  $A^T$ , where A is given in equation (2.58), and verify that the condition (2.62) must hold for the linear system to have solutions.

#### Exercise 2.4 (boundary conditions in byp codes)

- (a) Modify the m-file bvp2.m so that it implements a Dirichlet boundary condition at x = a and a Neumann condition at x = b and test the modified program.
- (b) Make the same modification to the m-file bvp4.m, which implements a fourth order accurate method. Again test the modified program.

#### Exercise 2.5 (accuracy on nonuniform grids)

In Example 1.4 a 3-point approximation to  $u''(x_i)$  is determined based on  $u(x_{i-1})$ ,  $u(x_i)$ , and  $u(x_{i+1})$  (by translating from  $x_1, x_2, x_3$  to general  $x_{i-1}, x_i$ , and  $x_{i+1}$ ). It is also determined that the truncation error of this approximation is  $\frac{1}{3}(h_{i-1}-h_i)u'''(x_i)+O(h^2)$ , where  $h_{i-1}=x_i-x_{i-1}$  and  $h_i=x_{i+1}-x_i$ , so the approximation is only first order accurate in h if  $h_{i-1}$  and  $h_i$  are O(h) but  $h_{i-1} \neq h_i$ .

The program bvp2.m is based on using this approximation at each grid point, as described in Example 2.3. Hence on a nonuniform grid the local truncation error is O(h) at each point, where h is some measure of the grid spacing (e.g., the average spacing on the grid). If we assume the method is stable, then we expect the global error to be O(h) as well as we refine the grid.

- (a) However, if you run bvp2.m you should observe second-order accuracy, at least provided you take a smoothly varying grid (e.g., set gridchoice = 'rtlayer' in bvp2.m). Verify this.
- (b) Suppose that the grid is defined by  $x_i = X(z_i)$  where  $z_i = ih$  for  $i = 0, 1, \ldots, m+1$  with h = 1/(m+1) is a uniform grid and X(z) is some smooth mapping of the interval [0,1] to the interval [a,b]. Show that if X(z) is smooth enough, then the local truncation error is in fact  $O(h^2)$ . Hint:  $x_i x_{i-1} \approx hX'(x_i)$ .
- (c) What average order of accuracy is observed on a random grid? To test this, set gridchoice = 'random' in bvp2.m and increase the number of tests done, e.g., by setting mvals = round(logspace(1,3,50)); to do 50 tests for values of m between 10 and 1000.

#### Exercise 2.6 (ill-posed boundary value problem)

Consider the following linear boundary value problem with Dirichlet boundary conditions:

$$u''(x) + u(x) = 0$$
 for  $a < x < b$   
 $u(a) = \alpha$ ,  $u(b) = \beta$ .

Note that this equation arises from a linearized pendulum, for example.

(a) Modify the m-file bvp2.m to solve this problem. Test your modified routine on the problem with

$$a=0, \quad b=1, \quad \alpha=2, \quad \beta=3.$$

Determine the exact solution for comparison.

- (b) Let a = 0 and  $b = \pi$ . For what values of  $\alpha$  and  $\beta$  does this boundary value problem have solutions? Sketch a family of solutions in a case where there are infinitely many solutions.
- (c) Solve the problem with

$$a = 0$$
,  $b = \pi$ ,  $\alpha = 1$ ,  $\beta = -1$ .

using your modified bvp2.m. Which solution to the boundary value problem does this appear to converge to as  $h \to 0$ ? Change the boundary value at  $b = \pi$  to  $\beta = 1$ . Now how does the numerical solution behave as  $h \to 0$ ?

(d) You might expect the linear system in part (c) to be singular since the boundary value problem is not well posed. It is not, because of discretization error. Compute the eigenvalues of the matrix A for this problem and show that an eigenvalue approaches 0 as  $h \to 0$ . Also show that  $||A^{-1}||_2$  blows up as  $h \to 0$  so that the discretization is unstable.

#### Exercise 2.7 (nonlinear pendulum)

- (a) Write a program to solve the boundary value problem for the nonlinear pendulum as discussed in the text. See if you can find yet another solution for the boundary conditions illustrated in Figures 2.4 and 2.5.
- (b) Find a numerical solution to this BVP with the same general behavior as seen in Figure 2.5 for the case of a longer time interval, say T=20, again with  $\alpha=\beta=0.7$ . Try larger values of T. What does  $\max_i \theta_i$  approach as T is increased? Note that for large T this solution exhibits "boundary layers".

## Chapter 3 Exercises

From: Finite Difference Methods for Ordinary and Partial Differential Equations by R. J. LeVeque, SIAM, 2007. http://www.amath.washington.edu/~rjl/fdmbook

#### Exercise 3.1 (code for Poisson problem)

The MATLAB script poisson.m solves the Poisson problem on a square  $m \times m$  grid with  $\Delta x = \Delta y = h$ , using the 5-point Laplacian. It is set up to solve a test problem for which the exact solution is  $u(x,y) = \exp(x+y/2)$ , using Dirichlet boundary conditions and the right hand side  $f(x,y) = 1.25 \exp(x+y/2)$ .

- (a) Test this script by performing a grid refinement study to verify that it is second order accurate.
- (b) Modify the script so that it works on a rectangular domain  $[a_x, b_x] \times [a_y, b_y]$ , but still with  $\Delta x = \Delta y = h$ . Test your modified script on a non-square domain.
- (c) Further modify the code to allow  $\Delta x \neq \Delta y$  and test the modified script.

#### Exercise 3.2 (9-point Laplacian)

- (a) Show that the 9-point Laplacian (3.17) has the truncation error derived in Section 3.5. **Hint:** To simplify the computation, note that the 9-point Laplacian can be written as the 5-point Laplacian (with known truncation error) plus a finite difference approximation that models  $\frac{1}{6}h^2u_{xxyy} + O(h^4)$ .
- (b) Modify the MATLAB script poisson.m to use the 9-point Laplacian (3.17) instead of the 5-point Laplacian, and to solve the linear system (3.18) where  $f_{ij}$  is given by (3.19). Perform a grid refinement study to verify that fourth order accuracy is achieved.

## Chapter 4 Exercises

From: Finite Difference Methods for Ordinary and Partial Differential Equations by R. J. LeVeque, SIAM, 2007. http://www.amath.washington.edu/~rjl/fdmbook

#### Exercise 4.1 (Convergence of SOR)

The m-file iter\_bvp\_Asplit.m implements the Jacobi, Gauss-Seidel, and SOR matrix splitting methods on the linear system arising from the boundary value problem u''(x) = f(x) in one space dimension.

- (a) Run this program for each method and produce a plot similar to Figure 4.2.
- (b) The convergence behavior of SOR is very sensitive to the choice of  $\omega$  (omega in the code). Try changing from the optimal  $\omega$  to  $\omega = 1.8$  or 1.95.
- (c) Let  $g(\omega) = \rho(G(\omega))$  be the spectral radius of the iteration matrix G for a given value of  $\omega$ . Write a program to produce a plot of  $g(\omega)$  for  $0 \le \omega \le 2$ .
- (d) From equations (4.22) one might be tempted to try to implement SOR as

```
for iter=1:maxiter
  uGS = (DA - LA) \ (UA*u + rhs);
  u = u + omega * (uGS - u);
  end
```

where the matrices have been defined as in iter\_bvp\_Asplit.m. Try this computationally and observe that it does not work well. Explain what is wrong with this and derive the correct expression (4.24).

#### Exercise 4.2 (Forward vs. backward Gauss-Seidel)

(a) The Gauss-Seidel method for the discretization of u''(x) = f(x) takes the form (4.5) if we assume we are marching forwards across the grid, for  $i = 1, 2, \ldots, m$ . We can also define a backwards Gauss-Seidel method by setting

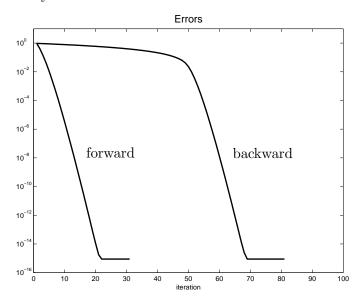
$$u_i^{[k+1]} = \frac{1}{2}(u_{i-1}^{[k]} + u_{i+1}^{[k+1]} - h^2 f_i), \quad \text{for } i = m, \ m-1, \ m-2, \ \dots, \ 1.$$
 (Ex4.2a)

Show that this is a matrix splitting method of the type described in Section 4.2 with M = D - U and N = L.

- (b) Implement this method in iter\_bvp\_Asplit.m and observe that it converges at the same rate as forward Gauss-Siedel for this problem.
- (c) Modify the code so that it solves the boundary value problem

$$\epsilon u''(x) = au'(x) + f(x), \qquad 0 \le x \le 1,$$
 (Ex4.2b)

with u(0) = 0 and u(1) = 0, where  $a \ge 0$  and the  $u'(x_i)$  term is discretized by the one-sided approximation  $(U_i - U_{i-1})/h$ . Test both forward and backward Gauss-Seidel for the resulting linear system. With a = 1 and  $\epsilon = 0.0005$ . You should find that they behave very differently:



Explain intuitively why sweeping in one direction works so much better than in the other.

**Hint:** Note that this equation is the steady equation for an advection-diffusion PDE  $u_t(x,t) + au_x(x,t) = \epsilon u_{xx}(x,t) - f(x)$ . You might consider how the methods behave in the case  $\epsilon = 0$ .

## Chapter 5 Exercises

From: Finite Difference Methods for Ordinary and Partial Differential Equations by R. J. LeVeque, SIAM, 2007. http://www.amath.washington.edu/~rjl/fdmbook

Exercise 5.1 (Uniqueness for an ODE)

Prove that the ODE

$$u'(t) = \frac{1}{t^2 + u(t)^2}, \text{ for } t \ge 1$$

has a unique solution for all time from any initial value  $u(1) = \eta$ .

Exercise 5.2 (Lipschitz constant for an ODE)

Let  $f(u) = \log(u)$ .

- (a) Determine the best possible Lipschitz constant for this function over  $2 \le u < \infty$ .
- (b) Is f(u) Lipschitz continuous over  $0 < u < \infty$ ?
- (c) Consider the initial value problem

$$u'(t) = \log(u(t)),$$
  
$$u(0) = 2.$$

Explain why we know that this problem has a unique solution for all  $t \ge 0$  based on the existence and uniqueness theory described in Section 5.2.1. (Hint: Argue that f is Lipschitz continuous in a domain that the solution never leaves, though the domain is not symmetric about  $\eta = 2$  as assumed in the theorem quoted in the book.)

Exercise 5.3 (Lipschitz constant for a system of ODEs)

Consider the system of ODEs

$$u_1' = 3u_1 + 4u_2,$$
  
$$u_2' = 5u_1 - 6u_2.$$

Determine the Lipschitz constant for this system in the max-norm  $\|\cdot\|_{\infty}$  and the 1-norm  $\|\cdot\|_1$ . (See Appendix A.3.)

Exercise 5.4 (Duhamel's principle)

Check that the solution u(t) given by (5.8) satisfies the ODE (5.6) and initial condition. Hint: To differentiate the matrix exponential you can differentiate the Taylor series (D.31) (in Appendix D) term by term.

Exercise 5.5 (matrix exponential form of solution)

The initial value problem

$$v''(t) = -4v(t),$$
  $v(0) = v_0,$   $v'(0) = v'_0$ 

has the solution  $v(t) = v_0 \cos(2t) + \frac{1}{2}v'_0 \sin(2t)$ . Determine this solution by rewriting the ODE as a first order system u' = Au so that  $u(t) = e^{At}u(0)$  and then computing the matrix exponential using (D.30) in Appendix D.

#### Exercise 5.6 (matrix exponential form of solution)

Consider the IVP

$$u_1' = 2u_1, u_2' = 3u_1 - u_2,$$

with initial conditions specified at time t = 0. Solve this problem in two different ways:

- (a) Solve the first equation, which only involves  $u_1$ , and then insert this function into the second equation to obtain a nonhomogeneous linear equation for  $u_2$ . Solve this using (5.8).
- (b) Write the system as u' = Au and compute the matrix exponential using (D.30) to obtain the solution.

#### Exercise 5.7 (matrix exponential for a defective matrix)

Consider the IVP

$$u_1' = 2u_1, u_2' = 3u_1 + 2u_2,$$

with initial conditions specified at time t=0. Solve this problem in two different ways:

- (a) Solve the first equation, which only involves  $u_1$ , and then insert this function into the second equation to obtain a nonhomogeneous linear equation for  $u_2$ . Solve this using (5.8).
- (b) Write the system as u' = Au and compute the matrix exponential using (D.35) to obtain the solution. (See Appendix C.3 for a discussion of the Jordan Canonical form in the defective case.)

#### Exercise 5.8 (Use of ode113 and ode45)

This problem can be solved by a modifying the m-files odesample.m and odesampletest.m available from the webpage.

Consider the third order initial value problem

$$v'''(t) + v''(t) + 4v'(t) + 4v(t) = 4t^{2} + 8t - 10,$$
  
$$v(0) = -3, \quad v'(0) = -2, \quad v''(0) = 2.$$

(a) Verify that the function

$$v(t) = -\sin(2t) + t^2 - 3$$

is a solution to this problem. How do you know it is the unique solution?

- (b) Rewrite this problem as a first order system of the form u'(t) = f(u(t), t) where  $u(t) \in \mathbb{R}^3$ . Make sure you also specify the initial condition  $u(0) = \eta$  as a 3-vector.
- (c) Use the MATLAB function ode113 to solve this problem over the time interval  $0 \le t \le 2$ . Plot the true and computed solutions to make sure you've done this correctly.
- (d) Test the MATLAB solver by specifying different tolerances spanning several orders of magnitude. Create a table showing the maximum error in the computed solution for each tolerance and the number of function evaluations required to achieve this accuracy.
- (e) Repeat part (d) using the MATLAB function ode45, which uses an embedded pair of Runge-Kutta methods instead of Adams-Bashforth-Moulton methods.

#### Exercise 5.9 (truncation errors)

Compute the leading term in the local truncation error of the following methods:

- (a) the trapezoidal method (5.22),
- (b) the 2-step BDF method (5.25),
- (c) the Runge-Kutta method (5.30).

#### Exercise 5.10 (Derivation of Adams-Moulton)

Determine the coefficients  $\beta_0$ ,  $\beta_1$ ,  $\beta_2$  for the third order, 2-step Adams-Moulton method. Do this in two different ways:

- (a) Using the expression for the local truncation error in Section 5.9.1,
- (b) Using the relation

$$u(t_{n+2}) = u(t_{n+1}) + \int_{t_{n+1}}^{t_{n+2}} f(u(s)) ds.$$

Interpolate a quadratic polynomial p(t) through the three values  $f(U^n)$ ,  $f(U^{n+1})$  and  $f(U^{n+2})$  and then integrate this polynomial exactly to obtain the formula. The coefficients of the polynomial will depend on the three values  $f(U^{n+j})$ . It's easiest to use the "Newton form" of the interpolating polynomial and consider the three times  $t_n = -k$ ,  $t_{n+1} = 0$ , and  $t_{n+2} = k$  so that p(t) has the form

$$p(t) = A + B(t+k) + C(t+k)t$$

where A, B, and C are the appropriate divided differences based on the data. Then integrate from 0 to k. (The method has the same coefficients at any time, so this is valid.)

#### Exercise 5.11 (Characteristic polynomials)

Determine the characteristic polynomials  $\rho(\zeta)$  and  $\sigma(\zeta)$  for the following linear multistep methods. Verify that (5.48) holds in each case.

- (a) The 3-step Adams-Bashforth method,
- (b) The 3-step Adams-Moulton method,
- (c) The 2-step Simpson's method of Example 5.16.

#### Exercise 5.12 (predictor-corrector methods)

- (a) Verify that the predictor-corrector method (5.51) is second order accurate.
- (b) Show that the predictor-corrector method obtained by predicting with the 2-step Adams-Bashforth method followed by correcting with the 2-step Adams-Moulton method is third order accurate.

#### Exercise 5.13 (Order of accuracy of Runge-Kutta methods)

Consider the Runge-Kutta methods defined by the tableaux below. In each case show that the method is third order accurate in two different ways: First by checking that the order conditions (5.35), (5.37), and (5.38) are satisfied, and then by applying one step of the method to  $u' = \lambda u$  and verifying that the Taylor series expansion of  $e^{k\lambda}$  is recovered to the expected order.

(a) Runge's 3rd order method:

(b) Heun's 3rd order method:

$$\begin{array}{c|cccc}
0 & & & \\
1/3 & 1/3 & & \\
2/3 & 0 & 2/3 & \\
& & 1/4 & 0 & \\
\end{array}$$

Exercise 5.14 (accuracy of TR-ZBDF2)

Use the approach suggested in the Remark at the bottom of page 129 to test the accuracy of the TR-BDF2 method (5.36).

#### Exercise 5.15 (Embedded Runge-Kutta method)

Consider the embedded Runge-Kutta method defined by the tableau below. Apply one step of this method to  $u' = \lambda u$  to obtain both  $U^{n+1}$  and  $\hat{U}^{n+1}$ . What is the order of accuracy of each method? What error estimate would be obtained when using this embedded method on this problem? How does it compare to the actual error in the lower order method? (Assume  $U^n$  is the exact value at time  $t_n$ ).

#### Exercise 5.16 (accuracy of a Runge-Kutta method)

- (a) Determine the leading term of the truncation error (i.e., the  $\mathcal{O}(k^2)$  term) for the Runge-Kutta method (5.30) of Example 5.11.
- (b) Do the same for the method (5.32) for the non-autonomous case.

#### Exercise 5.17 (R(z) for the trapezoidal method)

(a) Apply the trapezoidal method to the equation  $u' = \lambda u$  and show that

$$U^{n+1} = \left(\frac{1+z/2}{1-z/2}\right) U^n,$$

where  $z = \lambda k$ .

(b) Let

$$R(z) = \frac{1 + z/2}{1 - z/2}.$$

Show that  $R(z) = e^z + \mathcal{O}(z^3)$  and conclude that the one-step error of the trapezoidal method on this problem is  $\mathcal{O}(k^3)$  (as expected since the method is second order accurate).

Hint: One way to do this is to use the "Neumann series" expansion

$$\frac{1}{1-z/2} = 1 + \frac{z}{2} + \left(\frac{z}{2}\right)^2 + \left(\frac{z}{2}\right)^3 + \cdots$$

and then multiply this series by (1 + z/2). A more general approach to checking the accuracy of rational approximations to  $e^z$  is explored in the next exercises.

#### Exercise 5.18 (R(z) for Runge-Kutta methods)

Any r-stage Runge-Kutta method applied to  $u' = \lambda u$  will give an expression of the form

$$U^{n+1} = R(z)U^n$$

where  $z = \lambda k$  and R(z) is a rational function, a ratio of polynomials in z each having degree at most r. For an explicit method R(z) will simply be a polynomial of degree r and for an implicit method it will be a more general rational function.

Since  $u(t_{n+1}) = e^z u(t_n)$  for this problem, we expect that a pth order accurate method will give a function R(z) satisfying

$$R(z) = e^z + \mathcal{O}(z^{p+1})$$
 as  $z \to 0$ , (Ex5.18a)

as discussed in the Remark on page 129. The rational function R(z) also plays a role in stability analysis as discussed in Section 7.6.2.

One can determine the value of p in (Ex5.18a). by expanding  $e^z$  in a Taylor series about z = 0, writing the  $\mathcal{O}(z^{p+1})$  term as

$$Cz^{p+1} + \mathcal{O}(z^{p+2}),$$

multiplying through by the denominator of R(z), and then collecting terms. For example, for the trapezoidal method of Exercise 5.17,

$$\frac{1+z/2}{1-z/2} = \left(1+z+\frac{1}{2}z^2+\frac{1}{6}z^3+\cdots\right)+Cz^{p+1}+\mathcal{O}(z^{p+2})$$

gives

$$1 + \frac{1}{2}z = \left(1 - \frac{1}{2}z\right)\left(1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \cdots\right) + Cz^{p+1} + \mathcal{O}(z^{p+2})$$
$$= 1 + \frac{1}{2}z - \frac{1}{12}z^3 + \cdots + Cz^{p+1} + \mathcal{O}(z^{p+2})$$

and so

$$Cz^{p+1} = \frac{1}{12}z^3 + \cdots,$$

from which we conclude that p = 2.

(a) Let

$$R(z) = \frac{1 + \frac{1}{3}z}{1 - \frac{2}{3}z + \frac{1}{6}z^2}.$$

Determine p for this rational function as an approximation to  $e^z$ .

- (b) Determine R(z) and p for the backward Euler method.
- (c) Determine R(z) and p for the TR-BDF2 method (5.36).

#### Exercise 5.19 (Padé approximations)

A rational function R(z) = P(z)/Q(z) with degree m in the numerator and degree n in the denominator is called the (m,n) Padé approximation to a function f(z) if

$$R(z) - f(z) = \mathcal{O}(z^q)$$

with q as large as possible. The Padé approximation can be uniquely determined by expanding f(z) in a Taylor series about z = 0 and then considering the series

$$P(z) - Q(z)f(z),$$

collecting powers of z, and choosing the coefficients of P and Q to make as many terms vanish as possible. Trying to require that they all vanish will give a system of infintely many linear equations for the coefficients. Typically these can not all be satisfied simultaneously, while requiring the maximal number to hold will give a nonsingular linear system. (Note that the (m,0) Padé approximation is simply the first m+1 terms of the Taylor series.)

For this exercise, consider the exponential function  $f(z) = e^z$ .

(a) Determine the (1,1) Padé approximation of the form

$$R(z) = \frac{1 + a_1 z}{1 + b_1 z}.$$

Note that this rational function arises from the trapezoidal method applied to  $u' = \lambda u$  (see Exercise 5.18).

(b) Determine the (1,2) Padé approximation of the form

$$R(z) = \frac{1 + a_1 z}{1 + b_1 z + b_2 z^2}.$$

(c) Determine the (2,2) Padé approximation of the form

$$R(z) = \frac{1 + a_1 z + a_2 z^2}{1 + b_1 z + b_2 z^2}.$$

You can check your answers at http://mathworld.wolfram.com/PadeApproximant.html, for example.

Exercise 5.20 (R(z) for Runge-Kutta methods)

Consider a general r-stage Runge-Kutta method with tableau defined by an  $r \times r$  matrix A and a row vector  $b^T$  of length r. Let

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_r \end{bmatrix}, \qquad e = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}$$

and  $z = \lambda k$ .

(a) Show that if the Runge-Kutta method is applied to the equation  $u' = \lambda u$  the formulas (5.34) can be written concisely as

$$Y = U^n e + zAY,$$
  
$$U^{n+1} = U^n + zb^T Y.$$

and hence

$$U^{n+1} = (I + zb^{T}(I - zA)^{-1}e) U^{n}.$$
 (Ex5.20a)

(b) Recall that by Cramer's rule that if B is an  $r \times r$  matrix then the ith element of the vector  $y = B^{-1}e$  is given by

$$y_i = \frac{\det(B_i)}{\det(B)},$$

where  $B_i$  is the matrix B with the ith column replaced by e, and det denotes the determinant.

In the expression (Ex5.20a), B = I - zA and each element of B is linear in z. From the definition of the determinant it follows that det(B) will be a polynomial of degree at most r, while  $det(B_i)$  will be a polynomial of degree at most r - 1 (since the column vector e does does not involve z).

From these facts, conclude that (Ex5.20a) yields  $U^{n+1} = R(z)U^n$  where R(z) is a rational function of degree at most (r, r).

- (c) Explain why an explicit Runge-Kutta method (for which A is strictly lower triangular) results in R(z) being a polynomial of degree at most r (i.e., a rational function of degree at most (r,0)).
- (d) Use (Ex5.20a) to determine the function R(z) for the TR-BDF2 method (5.36). Note that in this case I zA is lower triangular and you can compute  $(I zA)^{-1}e$  by forward substitution. You should get the same result as in Exercise 5.18(c).

#### Exercise 5.21 (starting values)

In Example 5.18 it is claimed that generating a value  $U^1$  using the first order accurate forward Euler method and then computing using the midpoint method gives a method that is globally second order accurate. Check that this is true by implementing this approach in MATLAB for a simple ODE.

## Chapter 6 Exercises

From: Finite Difference Methods for Ordinary and Partial Differential Equations by R. J. LeVeque, SIAM, 2007. http://www.amath.washington.edu/~rjl/fdmbook

#### Exercise 6.1 (Lipschitz constant for a one-step method)

For the one-step method (6.17) show that the Lipschitz constant is  $L' = L + \frac{1}{2}kL^2$ .

#### Exercise 6.2 (Improved convergence proof for one-step methods)

The proof of convergence of 1-step methods in Section 6.3 shows that the global error goes to zero as  $k \to 0$ . However, this bound may be totally useless in estimating the actual error for a practical calculation.

For example, suppose we solve u' = -10u with u(0) = 1 up to time T = 10, so the true solution is  $u(T) = e^{-100} \approx 3.7 \times 10^{-44}$ . Using forward Euler with a time step k = 0.01, the computed solution is  $U^N = (.9)^{100} \approx 2.65 \times 10^{-5}$ , and so  $E^N \approx U^N$ . Since L = 10 for this problem, the error bound (6.16) gives

$$||E^N|| \le e^{100} \cdot 10 \cdot ||\tau||_{\infty} \approx 2.7 \times 10^{44} ||\tau||_{\infty}.$$
 (Ex6.2a)

Here  $\|\tau\|_{\infty} = |\tau^0| \approx 50k$ , so this upper bound on the error does go to zero as  $k \to 0$ , but obviously it is not a realistic estimate of the error. It is too large by a factor of about  $10^{50}$ .

The problem is that the estimate (6.16) is based on the Lipschitz constant  $L = |\lambda|$ , which gives a bound that grows exponentially in time even when the true and computed solutions are decaying exponentially.

- (a) Determine the computed solution and error bound (6.16) for the problem u' = 10u with u(0) = 1 up to time T = 10. Note that the error bound is the same as in the case above, but now it is a reasonable estimate of the actual error.
- (b) A more realistic error bound for the case where  $\lambda < 0$  can be obtained by rewriting (6.17) as

$$U^{n+1} = \Phi(U^n)$$

and then determining the Lipschitz constant for the function  $\Phi$ . Call this constant M. Prove that if  $M \leq 1$  and  $E^0 = 0$  then

$$|E^n| \leq T \|\tau\|_{\infty}$$

for  $nk \leq T$ , a bound that is similar to (6.16) but without the exponential term.

(c) Show that for forward Euler applied to  $u' = \lambda u$  we can take  $M = |1 + k\lambda|$ . Determine M for the case  $\lambda = -10$  and k = 0.01 and use this in the bound from part (b). Note that this is much better than the bound (Ex6.2a).

#### Exercise 6.3 (consistency and zero-stability of LMMs)

Which of the following Linear Multistep Methods are convergent? For the ones that are not, are they inconsistent, or not zero-stable, or both?

- (a)  $U^{n+2} = \frac{1}{2}U^{n+1} + \frac{1}{2}U^n + 2kf(U^{n+1})$
- (b)  $U^{n+1} = U^n$
- (c)  $U^{n+4} = U^n + \frac{4}{3}k(f(U^{n+3}) + f(U^{n+2}) + f(U^{n+1}))$
- (d)  $U^{n+3} = -U^{n+2} + U^{n+1} + U^n + 2k(f(U^{n+2}) + f(U^{n+1})).$

#### Exercise 6.4 (Solving a difference equation)

Consider the difference equation  $U^{n+2} = U^n$  with starting values  $U^0$  and  $U^1$ . The solution is clearly

$$U^n = \left\{ \begin{array}{ll} U^0 & \text{if } n \text{ is even,} \\ U^1 & \text{if } n \text{ is odd.} \end{array} \right.$$

Using the roots of the characteristic polynomial and the approach of Section 6.4.1, another representation of this solution can be found:

$$U^{n} = (U^{0} + U^{1}) + (U^{0} - U^{1})(-1)^{n}.$$

Now consider the difference equation  $U^{n+4} = U^n$  with four starting values  $U^0$ ,  $U^1$ ,  $U^2$ ,  $U^3$ . Use the roots of the characteristic polynomial to find an analogous representation of the solution to this equation.

#### Exercise 6.5 (Solving a difference equation)

(a) Determine the general solution to the linear difference equation  $2U^{n+3} - 5U^{n+2} + 4U^{n+1} - U^n = 0$ .

**Hint:** One root of the characteristic polynomial is at  $\zeta = 1$ .

- (b) Determine the solution to this difference equation with the starting values  $U^0 = 11$ ,  $U^1 = 5$ , and  $U^2 = 1$ . What is  $U^{10}$ ?
- (c) Consider the LMM

$$2U^{n+3} - 5U^{n+2} + 4U^{n+1} - U^n = k(\beta_0 f(U^n) + \beta_1 f(U^{n+1})).$$

For what values of  $\beta_0$  and  $\beta_1$  is local truncation error  $\mathcal{O}(k^2)$ ?

(d) Suppose you use the values of  $\beta_0$  and  $\beta_1$  just determined in this LMM. Is this a convergent method?

#### Exercise 6.6 (Solving a difference equation)

(a) Find the general solution of the linear difference equation

$$U^{n+2} - U^{n+1} + 0.25U^n = 0.$$

(b) Determine the particular solution with initial data  $U^0 = 2$ ,  $U^1 = 3$ . What is  $U^{10}$ ?

#### (c) Consider the iteration

$$\begin{bmatrix} U^{n+1} \\ U^{n+2} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -0.25 & 1 \end{bmatrix} \begin{bmatrix} U^n \\ U^{n+1} \end{bmatrix}.$$

The matrix appearing here is the "companion matrix" (D.19) for the above difference equation. If this matrix is called A, then we can determine  $U^n$  from the starting values using the nth power of this matrix. Compute  $A^n$  as discussed in Appendix D.2 and show that this gives the same solution found in part (b).

#### Exercise 6.7 (Convergence of backward Euler method)

Suppose the function f(u) is Lipschitz continuous over some domain  $|u-\eta| \le a$  with Lipschitz constant L. Let g(u) = u - kf(u) and let  $\Phi(v) = g^{-1}(v)$ , the inverse function.

Show that for k < 1/L, the function  $\Phi(v)$  is Lipschitz continuous over some domain  $|v - f(\eta)| \le b$  and determine a Lipschitz constant.

**Hint:** Suppose v = u - kf(u) and  $v^* = u^* - kf(u^*)$  and obtain an upper bound on  $|u - u^*|$  in terms of  $|v - v^*|$ .

Note: The backward Euler method (5.21) takes the form

$$U^{n+1} = \Phi(U^n)$$

and so this shows that the implicit backward Euler method is convergent.

#### Exercise 6.8 (Fibonacci sequence)

A Fibonacci sequence is generated by starting with  $F_0 = 0$  and  $F_1 = 1$  and summing the last two terms to get the next term in the sequence, so  $F_{n+1} = F_n + F_{n-1}$ .

- (a) Show that for large n the ratio  $F_n/F_{n-1}$  approaches the "golden ratio"  $\phi \approx 1.618034$ .
- (b) Show that the result of part (a) holds if any two integers are used as the starting values  $F_0$  and  $F_1$ , assuming they are not both zero.
- (c) Is this true for all real starting values  $F_0$  and  $F_1$  (not both zero)?

## Chapter 7 Exercises

From: Finite Difference Methods for Ordinary and Partial Differential Equations by R. J. LeVeque, SIAM, 2007. http://www.amath.washington.edu/~rjl/fdmbook

#### Exercise 7.1 (Convergence of midpoint method)

Consider the midpoint method  $U^{n+1} = U^{n-1} + 2kf(U^n)$  applied to the test problem  $u' = \lambda u$ . The method is zero-stable and second order accurate, and hence convergent. If  $\lambda < 0$  then the true solution is exponentially decaying.

On the other hand, for  $\lambda < 0$  and k > 0 the point  $z = k\lambda$  is never in the region of absolute stability of this method (see Example 7.7), and hence the numerical solution should be growing exponentially for any nonzero time step. (And yet it converges to a function that is exponentially decaying.)

Suppose we take  $U^0 = \eta$ , use Forward Euler to generate  $U^1$ , and then use the midpoint method for  $n = 2, 3, \ldots$  Work out the exact solution  $U^n$  by solving the linear difference equation and explain how the apparent paradox described above is resolved.

#### Exercise 7.2 (Example 7.10)

Perform numerical experiments to confirm the claim made in Example 7.10.

#### Exercise 7.3 (stability on a kinetics problem)

Consider the kinetics problem (7.8) with  $K_1 = 3$  and  $K_2 = 1$  and initial data  $u_1(0) = 3$ ,  $u_2(0) = 4$ , and  $u_3(0) = 2$  as shown in Figure 7.4. Write a program to solve this problem using the forward Euler method.

- (a) Choose a time step based on the stability analysis indicated in Example 7.12 and determine whether the numerical solution remains bounded in this case.
- (b) How large can you choose k before you observe instability in your program?
- (c) Repeat parts (a) and (b) for  $K_1 = 300$  and  $K_2 = 1$ .

#### Exercise 7.4 (damped linear pendulum)

The m-file ex7p11.m implements several methods on the damped linear pendulum system (7.11) of Example 7.11.

- (a) Modify the m-file to also implement the 2-step explicit Adams-Bashforth method AB2.
- (b) Test the midpoint, trapezoid, and AB2 methods (all of which are second order accurate) for each of the following case (and perhaps others of your choice) and comment on the behavior of each method.
  - (i) a = 100, b = 0 (undamped),
  - (ii) a = 100, b = 3 (damped),

(iii) a = 100, b = 10 (more damped).

#### Exercise 7.5 (fixed point iteration of implicit methods)

Let g(x) = 0 represent a system of s nonlinear equations in s unknowns, so  $x \in \mathbb{R}^s$  and  $g: \mathbb{R}^s \to \mathbb{R}^s$ . A vector  $\bar{x} \in \mathbb{R}^s$  is a fixed point of g(x) if

$$\bar{x} = g(\bar{x}).$$
 (Ex7.5a)

One way to attempt to compute  $\bar{x}$  is with fixed point iteration: from some starting guess  $x^0$ , compute

$$x^{j+1} = q(x^j) \tag{Ex7.5b}$$

for  $j = 0, 1, \dots$ 

- (a) Show that if there exists a norm  $\|\cdot\|$  such that g(x) is Lipschitz continuous with constant L < 1 in a neighborhood of  $\bar{x}$ , then fixed point iteration converges from any starting value in this neighborhood. **Hint:** Subtract equation (Ex7.5a) from (Ex7.5b).
- (b) Suppose g(x) is differentiable and let g'(x) be the  $s \times s$  Jacobian matrix. Show that if the condition of part (a) holds then  $\rho(g'(\bar{x})) < 1$ , where  $\rho(A)$  denotes the spectral radius of a matrix.
- (c) Consider a predictor-corrector method (see Section 5.9.4) consisting of forward Euler as the predictor and backward Euler as the corrector, and suppose we make N correction iterations, i.e., we set

$$\hat{U}^{0} = U^{n} + kf(U^{n}) 
\text{for } j = 0, 1, \dots, N - 1 
\hat{U}^{j+1} = U^{n} + kf(\hat{U}^{j}) 
\text{end} 
U^{n+1} = \hat{U}^{N}.$$

Note that this can be interpreted as a fixed point iteration for solving the nonlinear equation

$$U^{n+1} = U^n + kf(U^{n+1})$$

of the backward Euler method. Since the backward Euler method is implicit and has a stability region that includes the entire left half plane, as shown in Figure 7.1(b), one might hope that this predictor-corrector method also has a large stability region.

Plot the stability region  $S_N$  of this method for N=2, 5, 10, 20 (perhaps using plotS.m from the webpage) and observe that in fact the stability region does not grow much in size.

- (d) Using the result of part (b), show that the fixed point iteration being used in the predictor-corrector method of part (c) can only be expected to converge if  $|k\lambda| < 1$  for all eigenvalues  $\lambda$  of the Jacobian matrix f'(u).
- (e) Based on the result of part (d) and the shape of the stability region of Backward Euler, what do you expect the stability region  $S_N$  of part (c) to converge to as  $N \to \infty$ ?

## Chapter 8 Exercises

From: Finite Difference Methods for Ordinary and Partial Differential Equations by R. J. LeVeque, SIAM, 2007. http://www.amath.washington.edu/~rjl/fdmbook

#### Exercise 8.1 (stability region of TR-BDF2)

Use makeplotS.m from Chapter 7 to plot the stability region for the TR-BDF2 method (8.6). Observe that the method is L-stable.

#### Exercise 8.2 (Stiff decay process)

The mfile decay1.m uses ode113 to solve the linear system of ODEs arising from the decay process

$$A \stackrel{K_1}{\to} B \stackrel{K_2}{\to} C$$
 (Ex8.2a)

where  $u_1 = [A]$ ,  $u_2 = [B]$ , and  $u_3 = [C]$ , using  $K_1 = 1$ ,  $K_2 = 2$ , and initial data  $u_1(0) = 1$ ,  $u_2(0) = 0$ , and  $u_3(0) = 0$ .

- (a) Use decaytest.m to determine how many function evaluations are used for four different choices of tol.
- (b) Now consider the decay process

$$A \xrightarrow{K_1} D \xrightarrow{K_3} B \xrightarrow{K_2} C$$
 (Ex8.2b)

Modify the m-file decay1.m to solve this system by adding  $u_4 = [D]$  and using the initial data  $u_4 = 0$ . Test your modified program with a modest value of  $K_3$ , e.g.,  $K_3 = 3$ , to make sure it gives reasonable results and produces a plot of all 4 components of u.

- (c) Suppose  $K_3$  is much larger than  $K_1$  and  $K_2$  in (Ex8.2b). Then as A is converted to D, it decays almost instantly into C. In this case we would expect that  $u_4(t)$  will always be very small (though nonzero for t > 0) while  $u_j(t)$  for j = 1, 2, 3 will be nearly identical to what would be obtained by solving (Ex8.2a) with the same reaction rates  $K_1$  and  $K_2$ . Test this out by using  $K_3 = 1000$  and solving (Ex8.2b). (Using your modified m-file with ode113 and set tol=1e-6).
- (d) Test ode113 with  $K_3 = 1000$  and the four tolerances used in decaytest.m. You should observe two things:
  - (i) The number of function evaluations requires is much larger than when solving (Ex8.2a), even though the solution is essentially the same,
  - (ii) The number of function evaluations doesn't change much as the tolerance is reduced.

Explain these two observations.

(e) Plot the computed solution from part (d) with tol = 1e-2 and tol = 1e-4 and comment on what you observe.

- (f) Test your modified system with three different values of  $K_3 = 500$ , 1000 and 2000. In each case use tol = 1e-6. You should observe that the number of function evaluations needed grows linearly with  $K_3$ . Explain why you would expect this to be true (rather than being roughly constant, or growing at some other rate such as quadratic in  $K_3$ ). About how many function evaluations would be required if  $K_3 = 10^7$ ?
- (g) Repeat part (f) using ode15s in place of ode113. Explain why the number of function evaluations is much smaller and now roughly constant for large  $K_3$ . Also try  $K_3 = 10^7$ .

#### Exercise 8.3 (Stability region of RKC methods)

Use the m-file plotSrkc.m to plot the stability region for the second-order accurate s-stage Runge-Kutta-Chebyshev methods for r=3, 6 with damping parameter  $\epsilon=0.05$  and compare the size of these regions to those shown for the first-order accurate RKC methods in Figures 8.7 and 8.8.

#### Exercise 8.4 (Implicit midpoint method)

Consider the implicit Runge-Kutta method

$$U^* = U^n + \frac{k}{2}f(U^*, t_n + k/2),$$

$$U^{n+1} = U^n + kf(U^*, t_n + k/2).$$
(Ex8.4a)

The first step is Backward Euler to determine an approximation to the value at the midpoint in time and the second step is the midpoint method using this value.

- (a) Determine the order of accuracy of this method.
- (b) Determine the stability region.
- (c) Is this method A-stable? Is it L-stable?

#### Exercise 8.5 (The $\theta$ -method)

Consider the so-called  $\theta$ -method for u'(t) = f(u(t), t),

$$U^{n+1} = U^n + k[(1-\theta)f(U^n, t_n) + \theta f(U^{n+1}, t_{n+1})],$$
 (Ex8.5a)

where  $\theta$  is a fixed parameter. Note that  $\theta = 0, 1/2, 1$  all give familiar methods.

- (a) Show that this method is A-stable for  $\theta \geq 1/2$ .
- (b) Plot the stability region S for  $\theta = 0$ , 1/4, 1/2, 3/4, 1 and comment on how the stability region will look for other values of  $\theta$ .

## Chapter 9 Exercises

From: Finite Difference Methods for Ordinary and Partial Differential Equations by R. J. LeVeque, SIAM, 2007. http://www.amath.washington.edu/~rjl/fdmbook

#### Exercise 9.1 (leapfrog for heat equation)

Consider the following method for solving the heat equation  $u_t = u_{xx}$ :

$$U_i^{n+2} = U_i^n + \frac{2k}{h^2}(U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1}).$$

- (a) Determine the order of accuracy of this method (in both space and time).
- (b) Suppose we take  $k = \alpha h^2$  for some fixed  $\alpha > 0$  and refine the grid. For what values of  $\alpha$  (if any) will this method be Lax-Richtmyer stable and hence convergent?

**Hint:** Consider the MOL interpretation and the stability region of the time-discretization being used.

(c) Is this a useful method?

#### Exercise 9.2 (codes for heat equation)

- (a) The m-file heat\_CN.m solves the heat equation  $u_t = \kappa u_{xx}$  using the Crank-Nicolson method. Run this code, and by changing the number of grid points, confirm that it is second-order accurate. (Observe how the error at some fixed time such as T = 1 behaves as k and h go to zero with a fixed relation between k and h, such as k = 4h.)
  - You might want to use the function error\_table.m to print out this table and estimate the order of accuracy, and error\_loglog.m to produce a log-log plot of the error vs. h. See bvp\_2.m for an example of how these are used.
- (b) Modify heat\_CN.m to produce a new m-file heat\_trbdf2.m that implements the TR-BDF2 method on the same problem. Test it to confirm that it is also second order accurate. Explain how you determined the proper boundary conditions in each stage of this Runge-Kutta method.
- (c) Modify heat\_CN.m to produce a new m-file heat\_FE.m that implements the forward Euler explicit method on the same problem. Test it to confirm that it is  $\mathcal{O}(h^2)$  accurate as  $h \to 0$  provided when  $k = 24h^2$  is used, which is within the stability limit for  $\kappa = 0.02$ . Note how many more time steps are required than with Crank-Nicolson or TR-BDF2, especially on finer grids.
- (d) Test heat\_FE.m with  $k = 26h^2$ , for which it should be unstable. Note that the instability does not become apparent until about time 1.6 for the parameter values  $\kappa = 0.02$ , m = 39,  $\beta = 150$ . Explain why the instability takes several hundred time steps to appear, and why it appears as a sawtooth oscillation.

**Hint:** What wave numbers  $\xi$  are growing exponentially for these parameter values? What is the initial magnitude of the most unstable eigenmode in the given initial data? The expression (16.52) for the Fourier transform of a Gaussian may be useful.

#### Exercise 9.3 (heat equation with discontinuous data)

(a) Modify heat\_CN.m to solve the heat equation for  $-1 \le x \le 1$  with step function initial data

$$u(x,0) = \begin{cases} 1 & \text{if } x < 0 \\ 0 & \text{if } x \ge 0. \end{cases}$$
 (Ex9.3a)

With appropriate Dirichlet boundary conditions, the exact solution is

$$u(x,t) = \frac{1}{2}\operatorname{erfc}\left(x/\sqrt{4\kappa t}\right),$$
 (Ex9.3b)

where erfc is the complementary error function

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_{x}^{\infty} e^{-z^2} dz.$$

- (i) Test this routine m = 39 and k = 4h. Note that there is an initial rapid transient decay of the high wave numbers that is not captured well with this size time step.
- (ii) How small do you need to take the time step to get reasonable results? For a suitably small time step, explain why you get much better results by using m=38 than m=39. What is the observed order of accuracy as  $k\to 0$  when  $k=\alpha h$  with  $\alpha$  suitably small and m even?
- (b) Modify heat\_trbdf2.m (see Exercise 9.2) to solve the heat equation for  $-1 \le x \le 1$  with step function initial data as above. Test this routine using k = 4h and estimate the order of accuracy as  $k \to 0$  with m even. Why does the TR-BDF2 method work better than Crank-Nicolson?

#### Exercise 9.4 (Jacobi iteration as time stepping)

Consider the Jacobi iteration (4.4) for the linear system Au = f arising from a centered difference approximation of the boundary value problem  $u_{xx}(x) = f(x)$ . Show that this iteration can be interpreted as forward Euler time stepping applied to the MOL equations arising from a centered difference discretization of the heat equation  $u_t(x,t) = u_{xx}(x,t) - f(x)$  with time step  $k = \frac{1}{2}h^2$ .

Note that if the boundary conditions are held constant then the solution to this heat equation decays to the steady state solution that solves the boundary value problem. Marching to steady state with an explicit method is one way to solve the boundary value problem, though as we saw in Chapter 4 this is a very inefficient way to compute the steady state.

#### Exercise 9.5 (Diffusion and decay)

$$u_t = \kappa u_{xx} - \gamma u, \tag{Ex9.5a}$$

which models a diffusion with decay provided  $\kappa > 0$  and  $\gamma > 0$ . Consider methods of the form

$$U_{j}^{n+1} = U_{j}^{n} + \frac{k}{2h^{2}}[U_{j-1}^{n} - 2U_{j}^{n} + U_{j-1}^{n} + U_{j}^{n+1} - 2U_{j}^{n+1} + U_{j}^{n+1}] - k\gamma[(1-\theta)U_{j}^{n} + \theta U_{j}^{n+1}] \quad (\text{Ex}9.5\text{b})$$

where  $\theta$  is a parameter. In particular, if  $\theta = 1/2$  then the decay term is modeled with the same centered-in-time approach as the diffusion term and the method can be obtained by applying the Trapezoidal method to the MOL formulation of the PDE. If  $\theta = 0$  then the decay term is handled explicitly. For more general reaction-diffusion equations it may be advantageous to handle the reaction terms explicitly since these terms are generally nonlinear, so making them implicit would require solving nonlinear systems in each time step (whereas handling the diffusion term implicitly only gives a linear system to solve in each time step).

- (a) By computing the local truncation error, show that this method is  $\mathcal{O}(k^p + h^2)$  accurate, where p = 2 if  $\theta = 1/2$  and p = 1 otherwise.
- (b) Using von Neumann analysis, show that this method is unconditionally stable if  $\theta \geq 1/2$ .
- (c) Show that if  $\theta = 0$  then the method is stable provided  $k \leq 2/\gamma$ , independent of h.

## Chapter 10 Exercises

From: Finite Difference Methods for Ordinary and Partial Differential Equations by R. J. LeVeque, SIAM, 2007. http://www.amath.washington.edu/~rjl/fdmbook

#### Exercise 10.1 (One-sided and centered methods)

Let  $U = [U_0, U_1, \dots, U_m]^T$  be a vector of function values at equally spaced points on the interval  $0 \le x \le 1$ , and suppose the underlying function is periodic and smooth. Then we can approximate the first derivative  $u_x$  at all of these points by DU, where D is circulant matrix such as

$$D_{-} = \frac{1}{h} \begin{bmatrix} 1 & & & -1 \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & -1 & 1 & \\ & & & -1 & 1 \end{bmatrix}, \qquad D_{+} = \frac{1}{h} \begin{bmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & -1 & 1 & \\ & & & -1 & 1 \\ 1 & & & & -1 \end{bmatrix}$$
(Ex10.1a)

for first-order accurate one-sided approximations or

$$D_0 = \frac{1}{2h} \begin{bmatrix} 0 & 1 & & -1 \\ -1 & 0 & 1 & & \\ & -1 & 0 & 1 & \\ & & -1 & 0 & 1 \\ 1 & & & -1 & 0 \end{bmatrix}$$
 (Ex10.1b)

for a second-order accurate centered approximation. (These are illustrated for a grid with m+1=5 unknowns and h=1/5.)

The advection equation  $u_t + au_x = 0$  on the interval  $0 \le x \le 1$  with periodic boundary conditions gives rise to the MOL discretization U'(t) = -aDU(t) where D is one of the matrices above.

(a) Discretizing  $U' = -aD_{-}U$  by forward Euler gives the first order upwind method

$$U_j^{n+1} = U_j^n - \frac{ak}{h}(U_j^n - U_{j-1}^n),$$
 (Ex10.1c)

where the index i runs from 0 to m with addition of indices performed mod m+1 to incorporate the periodic boundary conditions.

Suppose instead we discretize the MOL equation by the second-order Taylor series method,

$$U^{n+1} = U^n - akD_-U^n + \frac{1}{2}(ak)^2D_-^2U^n.$$
 (Ex10.1d)

Compute  $D_{-}^{2}$  and also write out the formula for  $U_{i}^{n}$  that results from this method.

(b) How accurate is the method derived in part (a) compared to the Beam-Warming method, which is also a 3-point one-sided method?

(c) Suppose we make the method (Ex10.1c) more symmetric:

$$U^{n+1} = U^n - \frac{ak}{2}(D_+ + D_-)U^n + \frac{1}{2}(ak)^2 D_+ D_- U^n.$$
 (Ex10.1e)

Write out the formula for  $U_j^n$  that results from this method. What standard method is this?

#### Exercise 10.2 (Eigenvalues of $A_{\epsilon}$ for upwind)

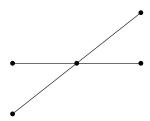
- (a) Produce a plot similar to those shown in Figure 10.1 for the upwind method (10.21) with the same values of a = 1, h = 1/50 and k = 0.8h used in that figure.
- (b) Produce the corresponding plot if the one-sided method (10.22) is instead used with the same values of a, h, and k.

#### Exercise 10.3 (skewed leapfrog)

Suppose a > 0 and consider the following skewed leapfrog method for solving the advection equation  $u_t + au_x = 0$ :

$$U_j^{n+1} = U_{j-2}^{n-1} - \left(\frac{ak}{h} - 1\right) (U_j^n - U_{j-2}^n).$$
 (Ex10.3a)

The stencil of this method is



Note that if  $ak/h \approx 1$  then this stencil roughly follows the characteristic of the advection equation and might be expected to be more accurate than standard leapfrog. (If ak/h = 1 the method is exact.)

- (a) What is the order of accuracy of this method?
- (b) For what range of Courant number ak/h does this method satisfy the CFL condition?
- (c) Show that the method is in fact stable for this range of Courant numbers by doing von Neumann analysis. **Hint:** Let  $\gamma(\xi) = e^{i\xi h}g(\xi)$  and show that  $\gamma$  satisfies a quadratic equation closely related to the equation (10.34) that arises from a von Neumann analysis of the leapfrog method.

#### Exercise 10.4 (trapezoid method for advection)

Consider the method

$$U_j^{n+1} = U_j^n - \frac{ak}{2h}(U_j^n - U_{j-1}^n + U_j^{n+1} - U_{j-1}^{n+1}).$$
 (Ex10.4a)

for the advection equation  $u_t + au_x = 0$  on  $0 \le x \le 1$  with periodic boundary conditions.

- (a) This method can be viewed as the trapezoidal method applied to an ODE system U'(t) = AU(t) arising from a method of lines discretization of the advection equation. What is the matrix A? Don't forget the boundary conditions.
- (b) Suppose we want to fix the Courant number ak/h as  $k, h \to 0$ . For what range of Courant numbers will the method be stable if a > 0? If a < 0? Justify your answers in terms of eigenvalues of the matrix A from part (a) and the stability regions of the trapezoidal method.
- (c) Apply von Neumann stability analysis to the method (Ex10.4a). What is the amplification factor  $q(\xi)$ ?
- (d) For what range of ak/h will the CFL condition be satisfied for this method (with periodic boundary conditions)?
- (e) Suppose we use the same method (Ex10.4a) for the initial-boundary value problem with  $u(0,t) = g_0(t)$  specified. Since the method has a one-sided stencil, no numerical boundary condition is needed at the right boundary (the formula (Ex10.4a) can be applied at  $x_{m+1}$ ). For what range of ak/h will the CFL condition be satisfied in this case? What are the eigenvalues of the A matrix for this case and when will the method be stable?

#### Exercise 10.5 (modified equation for Lax-Wendroff)

Derive the modified equation (10.45) for the Lax-Wendroff method.

#### Exercise 10.6 (modified equation for Beam-Warming)

Show that the Beam-Warming method (10.26) is second order accurate on the advection equation and also derive the modified equation (10.47) on which it is third order accurate.

#### Exercise 10.7 (modified equation for trapezoidal)

Determine the modified equation on which the method

$$U_j^{n+1} = U_j^n - \frac{ak}{2h}(U_j^n - U_{j-1}^n + U_j^{n+1} - U_{j-1}^{n+1}).$$

from Exercise 10.4 is second order accurate. Is this method predominantly dispersive or dissipative?

#### Exercise 10.8 (computing with Lax-Wendroff and upwind)

The m-file advection\_LW\_pbc.m implements the Lax-Wendroff method for the advection equation on  $0 \le x \le 1$  with periodic boundary conditions.

- (a) Observe how this behaves with m+1=50, 100, 200 grid points. Change the final time to tfinal = 0.1 and use the m-files error\_table.m and error\_loglog.m to verify second order accuracy.
- (b) Modify the m-file to create a version advection\_up\_pbc.m implementing the upwind method and verify that this is first order accurate.
- (c) Keep m fixed and observe what happens with advection\_up\_pbc.m if the time step k is reduced, e.g. try k=0.4h, k=0.2h, k=0.1h. When a convergent method is applied to an ODE we expect better accuracy as the time step is reduced and we can view the upwind method as an ODE solver applied to an MOL system. However, you should observe decreased accuracy as  $k \to 0$  with h fixed. Explain this apparent paradox. **Hint:** What ODE system are we solving more accuracy? You might also consider the modified equation (10.44).

#### Exercise 10.9 (computing with leapfrog)

The m-file advection\_LW\_pbc.m implements the Lax-Wendroff method for the advection equation on  $0 \le x \le 1$  with periodic boundary conditions.

- (a) Modify the m-file to create a version advection\_lf\_pbc.m implementing the leapfrog method and verify that this is second order accurate. Note that you will have to specify two levels of initial data. For the convergence test set  $U_j^1 = u(x_j, k)$ , the true solution at time k.
- (b) Modify advection\_lf\_pbc.m so that the initial data consists of a wave packet

$$\eta(x) = \exp(-\beta(x - 0.5)^2)\sin(\xi x)$$
 (Ex10.9a)

Work out the true solution u(x,t) for this data. Using  $\beta = 100$ ,  $\xi = 80$  and  $U_j^1 = u(x_j,k)$ , test that your code still exhibits second order accuracy for k and h sufficiently small.

(c) Using  $\beta = 100$ ,  $\xi = 150$  and  $U_j^1 = u(x_j, k)$ , estimate the group velocity of the wave packet computed with leapfrog using m = 199 and k = 0.4h. How well does this compare with the value (10.52) predicted by the modified equation?

#### Exercise 10.10 (Lax-Richtmyer stability of leapfrog as a one-step method)

Consider the leapfrog method for the advection equation  $u_t + au_x = 0$  on  $0 \le x \le 1$  with periodic boundary conditions. From the von Neumann analysis of Example 10.4 we expect this method to be stable for |ak/h| < 1. However, the Lax Equivalence theorem as stated in Section 9.5 only applies to 1-step (2-level) methods. The point of this exercise is to show that the 3-level leapfrog method can be interpreted as a 1-step method to which the Lax Equivalence theorem applies.

The leapfrog method  $U^{n+1} = U^{n-1} + 2kAU^n$  can be rewritten as

$$\begin{bmatrix} U^{n+1} \\ U^n \end{bmatrix} = \begin{bmatrix} 2kA & I \\ I & 0 \end{bmatrix} \begin{bmatrix} U^n \\ U^{n-1} \end{bmatrix},$$
 (Ex10.10a)

which has the form  $V^{n+1} = BV^n$ .

(a) Show that the matrix B defined by (Ex10.10a) has 2(m+1) eigenvectors of the form

$$\begin{bmatrix} g_p^- u^p \\ u^p \end{bmatrix}, \quad \begin{bmatrix} g_p^+ u^p \\ u^p \end{bmatrix}, \quad \text{for } p = 1, 2, \dots, m+1, \tag{Ex10.10b}$$

where  $u^p \in \mathbb{R}^{m+1}$  are the eigenvectors of A given by (10.12) and  $g_p^{\pm}$  are the two roots of a quadratic equation. Explain how this quadratic equation relates to (10.34) (what values of  $\xi$  are relevant for this grid?)

What are the eigenvalues of B?

(b) Show that if

$$|ak/h| < 1 \tag{Ex10.10c}$$

then the eigenvalues of B are distinct with magnitude equal to 1.

(c) The result of part (b) is not sufficient to prove that leapfrog is Lax-Ricthmyer stable. The matrix B is not normal and the matrix of right eigenvectors R with columns given by (Ex10.10b) is not unitary. By (D.8) in Appendix D we have

$$||B^n||_2 \le ||R||_2 ||R^{-1}||_2 = \kappa_2(R).$$
 (Ex10.10d)

To prove uniform power boundedness and stability we must show that the condition number of R is uniformly bounded as  $k \to 0$  provided (Ex10.10c) is satisfied.

Prove this by the following steps:

(i) Let

$$U = \frac{1}{\sqrt{m+1}} \begin{bmatrix} u^1 & u^2 & \cdots & u^p \end{bmatrix} \in \mathbb{R}^{(m+1)\times(m+1)}$$
 (Ex10.10e)

be an appropriately scaled right eigenvector matrix of A. Show that with this scaling, U is a unitary matrix:  $U^HU = I$ .

(ii) Show that the right eigenvector matrix of B can be written as

$$R = \begin{bmatrix} UG^{-} & UG^{+} \\ U & U \end{bmatrix}$$
 (Ex10.10f)

where  $G^{\pm} = \text{diag}(g_1^{\pm}, \ldots, g_{m+1}^{\pm}).$ 

- (iii) Show that if  $x = \begin{bmatrix} x \\ y \end{bmatrix} \in \mathbb{R}^{2(m+1)}$  has  $||z||_2 = 1$  then  $||Rz||_2 \leq C$  for some constant independent of m, and hence  $||R||_2 \leq C$  for all k. (It is fairly easy to show this with  $C = 2\sqrt{2}$  and with a bit more work that in fact  $||R||_2 = 2$  for all k.)
- (iv) Let

$$L = \begin{bmatrix} G^{-}U^{H} & U^{H} \\ G^{+}U^{H} & U^{H} \end{bmatrix}.$$
 (Ex10.10g)

Show that LR is a diagonal matrix and hence  $R^{-1}$  is a diagonal scaling of the matrix L. Determine  $R^{-1}$ .

(v) Use the previous result to show that

$$||R^{-1}||_2 \le \frac{C}{1-\nu^2}$$
 (Ex10.10h)

for some constant C, where  $\nu = ak/h$  is the Courant number.

- (vi) Conclude from the above steps that B is uniformly power bounded and hence the leapfrog method is Lax-Richtmyer stable provided that  $|\nu| < 1$ .
- (d) Show that the leapfrog method with periodic boundary conditions is also stable in the case |ak/h| = 1 if m+1 is not divisible by 4. Find a good set of initial data  $U^0$  and  $U^1$  to illustrate the instability that arises if m+1 is divisible by 4 and perform a calculation that demonstrates nonconvergence in this case.

#### Exercise 10.11 (Modified equation for Gauss-Seidel)

Exercise 9.4 illustrates how the Jacobi iteration for solving the boundary value problem  $u_{xx}(x) = f(x)$  can be viewed as an explicit time-stepping method for the heat equation  $u_t(x,t) = u_{xx}(x,t) - f(x)$  with a time step  $k = h^2/2$ .

Now consider the Gauss-Seidel method for solving the linear system,

$$U_j^{n+1} = \frac{1}{2}(U_{j-1}^{n+1} + U_{j+1}^n - h^2 f(x_j)).$$
 (Ex10.11a)

This can be viewed as a time stepping method for some PDE. Compute the modified equation for this finite difference method and determine what PDE it is consistent with if we let  $k = h^2/2$  again. Comment on how this relates to the observation in Section 4.2.1 that Gauss-Seidel takes roughly half as many iterations as Jacobi to converge.

## Chapter 11 Exercises

From: Finite Difference Methods for Ordinary and Partial Differential Equations by R. J. LeVeque, SIAM, 2007. http://www.amath.washington.edu/~rjl/fdmbook

#### Exercise 11.1 (two-dimensional Lax-Wendroff)

(a) Derive the two-dimensional Lax-Wendroff method from (11.6) by using standard centered approximations to  $u_x$ ,  $u_y$ ,  $u_{xx}$  and  $u_{yy}$  and the approximation

$$u_{xy}(x_i, y_j) \approx \frac{1}{4h^2} \left[ (U_{i+1,j+1} - U_{i-1,j+1}) - (U_{i+1,j-1} - U_{i-1,j-1}) \right].$$
 (Ex11.1a)

(b) Compute the leading term of the truncation error to show that this method is second order accurate.

#### Exercise 11.2 (Strang splitting)

(a) Show that the Strang splitting is second order accurate on the problem (11.18) by comparing

$$\exp\left(\frac{1}{2}Ak\right)\exp(Bk)\exp\left(\frac{1}{2}Ak\right)$$
 (Ex11.2a)

with (11.22).

(b) Show that second order accuracy on (11.18) can also be achieved by alternating the splitting (11.17) in even numbered time steps with

$$U^* = \mathcal{N}_B(U^n, k),$$
  

$$U^{n+1} = \mathcal{N}_A(U^*, k)$$
(Ex11.2b)

in odd numbered times steps.

#### Exercise 11.3 (accuracy of IMEX method)

Compute the truncation error of the method (11.26) and confirm that it is second order accurate.