1. **Numerical Differentiation.** Find the best approximation to the second derivative $d^2 f(x)/dx^2$ at $x = x_j$ of a function $f(x)$ using (a) the Taylor series approach and (b) the interpolating polynomial approach given $f$ values at

(a) $x_j - h, x_j$ and $x_j + h$ (centre formula),
(b) $x_j - 2h, x_j - h$ and $x_j$ (left-sided formula),
(c) $x_j, x_j + h$ and $x_j + 2h$ (right-sided formula),
(d) $x_j, x_j + h, x_j + 2h$ and $x_j + 3h$ (right-sided formula),
(e) $x_j - \lambda h, x_j$ and $x_j + h$ (non-uniform grid).

In each case, state what the order of accuracy of the formula is in terms of $h$.

2. **Polynomial Interpolation.** Examine how polynomial interpolation over an uniform grid can go wrong by playing with the following MATLAB code which considers $f(x) := 1/(1 + 16x^2)$ over $[-1, 1]$. Try $N = 5, 10, 15, 20$ and different functions which are regular over the real line segment $[-1, 1]$ but have singularities nearby in the complex plane. Then try another function which is analytic like $f(x) := e^x$ (although MATLAB’s interpolation function may struggle if $N$ is too large!). Confirm interpolation over (non-uniform) Chebyshhev points always works well.

```matlab
% Matlab program: Polynomial Interpolation
N=10;
xx=-1.01:0.005:1.01;
for i=1:2
  if i==1, s='equispaced pts'; x=-1+2*(0:N)/N; end
  if i==2, s='Chebyshev pts';  x=cos(pi*(0:N)/N); end
  subplot(2,1,i)
  % change function in the next two lines
  u =1./(1+16*x.^2);
  uu=1./(1+16*xx.^2);
  p=polyfit(x,u,N);  % calculate interpolating poly.
  pp=polyval(p,xx);  % evaluate poly over dense grid
  % plot interpolant over equispaced grid
  plot(x,u,'.b','markersize',13)
  hold on
  plot(xx,pp,'-b')
  plot(xx,uu,'-r')
  axis([-1.1 1.1 -1 1.5]); title(s)
  error=norm(uu-pp,inf);
```
3. **ODE revision: Order of Accuracy.** If $L$ is a nonzero integer, the initial value ODE problem

$$u_t(t) = f(u, t) := \frac{L}{t+1} u(t), \quad u(0) = 1$$

has a unique solution $u(t) = (t+1)^{L}$. Suppose we calculate an approximation to $u(2)$ using the following methods

(a) $u^{n+1} = u^n + kf^n$ (Euler’s Method)
(b) $u^{n+1} = u^{n-1} + 2kf^n$ (Midpoint rule)
(c) $u^{n+1} = u^n + \frac{k}{12}(55f^n - 59f^{n-1} + 37f^{n-2} - 9f^{n-3})$ (higher order Adams-Bashforth method)

(using exact values where needed for initialisation). Find the order of accuracy of the methods and hence identify the maximum value of $L$ for which each will produce the *exact* solution.

4. **ODE revision: Stability Analysis.** By the method of undetermined coefficients, show that the best formula of the form

$$u^{n+1} = \alpha u^n + \beta u^{n-1} + k(\gamma f^n + \delta f^{n-1})$$

for integrating the ODE $u_t = f(u, t)$ is

$$u^{n+1} = -4u^n + 5u^{n-1} + k(4f^n + 2f^{n-1})$$

and that it has an order of accuracy of 3. Then show using von Neumann analysis (where you substitute in the infinite wavelength ‘ODE version’ $u^n = g^n$ of $u^n_j = g(\xi)^n \exp(i\xi jh)$) that the formula is unstable in the limit of $k \to 0$ and therefore useless.

5. **ODE revision: Stability Analysis.** Consider the first order accurate integration strategy

$$u^{n+1} = 2u^n - u^{n-1}$$

for the ODE $u_t = f(u, t)$. Why can’t this formula possibly work (i.e. produce convergent approximations)? Show that it is unstable.

6. **ODE revision: Convergence.** Which of the following formulae for integrating the ODE $u_t = f(u, t)$ are convergent? Are the nonconvergent ones inconsistent or unstable or both?

(a) $u^{n+1} = \frac{1}{2}u^n + \frac{1}{2}u^{n-1} + 2kf^n$
(b) $u^{n+1} = u^n$
(c) $u^{n+4} = u^n + \frac{4}{3}(f^{n+3} + f^{n+2} + f^{n+1})$
(d) $u^{n+3} = u^{n+1} + \frac{1}{3}k(7f^{n+2} - 2f^{n+1} + f^n)$
7. **Parabolic PDEs.** Find the order of accuracy and the stability restriction on \( \mu := k/h^2 \) (\( k = \) time step and \( h = \) space step) of the following finite difference methods to integrate the heat equation \( u_t = u_{xx} \)

(a) \( u_j^{n+1} = u_j^n + \mu(u_{j+1}^n - 2u_j^n + u_{j-1}^n) \) (Euler’s Method)

(b) \( u_j^{n+1} = u_j^n + \mu(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}) \) (Backward Euler)

(c) \( u_j^{n+1} = u_j^n + \frac{1}{2}\mu(u_{j+1}^n - 2u_j^n + u_{j-1}^n) + \frac{1}{2}\mu(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}) \) (Crank-Nicolson method)

(d) \( u_j^{n+1} = u_j^{n-1} + 2\mu(u_{j+1}^n - 2u_j^n + u_{j-1}^n) \) (Leapfrog method)

[Note the general form]

\[ u_j^{n+1} = u_j^n + (1 - \theta)\mu(u_{j+1}^n - 2u_j^n + u_{j-1}^n) + \theta\mu(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}) \]

for \( 0 \leq \theta \leq 1 \) has the special cases \( \theta = 0 \) (Euler’s method), \( \theta = 1/2 \) (Crank-Nicolson) and \( \theta = 1 \) (backward Euler).

8. **Parabolic PDEs.** For solving the nonlinear heat equation \( u_t = (a(u)u_x)_x \) consider the explicit scheme

\[ u_{j+1}^{n+1} = u_j^n + \mu[a_{j+1/2}^n(u_{j+1}^n - u_j^n) - a_{j-1/2}^n(u_{j}^n - u_{j-1}^n)] \]

where \( a_{j+1/2}^n := \frac{1}{2}a(u_{j}^n + a(u_{j+1}^n)) \) and \( \mu := k/h^2 \). If \( 0 < a_x \leq a(u) \leq a^* \), apply von Neumann analysis by freezing the nonlinear coefficient to determine a reasonable condition on \( \mu \) for stability.

9. **Parabolic PDEs.** Consider the advection-diffusion equation

\[ u_t + au_x - u_{xx} = 0 \]

with Dirichlet b.c.s and \( a \geq 0 \) a constant. Show that

\[ u(x, t) = \exp[-(il\pi a + (l\pi)^2)t + il\pi x] \]

is a set of particular solutions of the problem. Use von Neumann analysis to derive the stability condition for the Upwind scheme

\[ \frac{u_j^{n+1} - u_j^n}{k} + a \frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{h} = \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{h^2}. \]

What is the order of accuracy of the scheme?

10. **Hyperbolic PDEs.** Determine the coefficients \( c_0, c_1 \) and \( c_{-1} \) so that the scheme

\[ u_j^{n+1} = c_{-1}u_{j-1}^n + c_0u_j^n + c_1u_{j+1}^n \]

for the solution of \( u_t + au_x = 0 \) agrees with the Taylor series expansion of \( u(x_j, t_{n+1}) \) to as high an order as possible when \( a \) is a positive constant. Verify that the result is the Lax-Wendroff scheme.

In the same way determine the coefficients in the scheme

\[ u_j^{n+1} = d_{-2}u_{j-2}^n + d_{-1}u_{j-1}^n + d_0u_j^n. \]

Verify that the coefficients \( d \) correspond to the coefficients \( c \) in the Lax-Wendroff scheme but with \( \nu := ak/h \) replaced by \( \nu - 1 \). Explain why this is so, by making the change of variable \( \xi = x - \lambda t \) in the differential equation where \( \lambda = h/k \). Hence, or otherwise, find the stability conditions for the scheme.
11. **Hyperbolic PDEs.** For the equation \( u_t = u_x \) all information propagates leftward at a speed 1, and so the mathematical domain of dependence for the point \((x, t)\) is the line \((x + T, t - T)\) for \(T > 0\). Use the CFL condition to derive a necessary condition for stability of the Euler method

\[
u_{j}^{n+1} - u_{j}^{n} = \frac{1}{2}\lambda(u_{j+1}^{n} - u_{j-1}^{n})
\]

and Lax-Wendroff scheme

\[
u_{j}^{n+1} - u_{j}^{n} = \frac{1}{2}\lambda(u_{j+1}^{n} - u_{j-1}^{n}) + \frac{1}{2}\lambda^2(u_{j+1}^{n} - 2u_{j}^{n} + u_{j-1}^{n})
\]

where \(\lambda := k/h\). Show using von Neumann analysis that the CFL condition is also sufficient for one scheme but not for the other. For more examples see [1] p169.

12. **Hyperbolic PDEs.** For the linear advection equation \( u_t + au_x = 0 \) \((a \text{ a positive constant})\), a generalised upwind scheme on a uniform mesh is defined by

\[
u_{j}^{n+1} = (1 - \theta)u_{j}^{n} + \theta u_{k-1}^{n}
\]

where \(x_{k} - \theta h = x_{j} - ak\) and \(0 \leq \theta < 1\). Verify that the CFL condition requires no restriction on \(k\) and that von Neumann stability analysis also shows that stability is unrestricted. What is the truncation error of the scheme, and how does it behave as \(k\) increases?

13. **Hyperbolic PDEs.** Derive an explicit central difference scheme for the solution of

\[u_{xx} - (1 + 4x)^2u_{tt} = 0\]

on the region \(0 < x < 1\) and \(t > 0\) given

\[u(x, 0) = x^2, \quad u_t(x, 0) = 0, \quad u_x(0, t) = 0, \quad u(1, t) = 1.\]

Show how the boundary conditions are included in the numerical scheme. Find the characteristics of the differential equation and use the CFL condition to derive a stability restriction.

14. **Hyperbolic PDEs.** Consider the implicit scheme

\[
u_{j}^{n+1} - u_{j}^{n} = \frac{k}{2}u_{j+1}^{n+1} - u_{j-1}^{n+1}
\]

for solving \(u_t + au_x = 0\) where \(a\) is a positive constant. Use von Neumann analysis to prove that the amplification factor \(g(\xi)\) for the scheme is \(1/(1 + ia\mu \sin \xi h)\) where \(\mu := k/h\) and hence that the scheme is unconditionally stable. Describe the corresponding dissipation and dispersion errors for the scheme.

15. **Hyperbolic PDEs.** The linearised 1-D forms of the isentropic compressible fluid flow equations are

\[
\begin{align*}
\rho_t + q\rho_x + w_x & = 0, \\
w_t + qw_x + a^2 \rho_x & = 0,
\end{align*}
\]

where \(a\) and \(q\) are positive constants. Show that an explicit scheme which uses central differences for the \(x\)-derivatives is always unstable. By adding the extra terms arising from the Lax-Wendroff scheme, derive a conditionally stable scheme and find the stability condition.
16. **Dissipation.** Determine whether each of the following models of \( u_t = u_x \) is non-dissipative, dissipative or neither. If dissipative, determine the order of dissipativity.

(a) \( u_j^{n+1} = u_j^n + \frac{1}{2}\lambda(u_j^{n+1} - u_{j-1}^n) + \frac{1}{2}\lambda^2(u_{j+1}^n - 2u_j^n + u_{j-1}^n) \) \ (Lax-Wendroff)

(b) \( u_j^{n+1} = u_j^n + \frac{1}{2}\lambda(u_{j+1}^{n+1} - u_{j-1}^n) \) \ (Backward Euler)

(c) \( u_j^{n+1} = u_j^n + \lambda(u_{j+1}^n - u_j^n) \) \ (Upwind)

(d) \( u_j^{n+1} = u_j^{n-1} + \frac{\lambda}{2}(u_{j+1}^n - u_j^n) - \frac{\lambda}{2}(u_{j+1}^n - u_{j-1}^n) \) \ (4th order Leapfrog)

where \( \lambda := k/h \).

17. **Dispersion.** Calculate and plot the dispersion relation for the Crank-Nicolson model of \( u_t = iu_{xx} \), the Schrödinger equation. Calculate the group velocity. How does this compare to the true group velocity?

18. **Boundary Conditions.** The leap frog model for \( u_t = u_x \) is

\[
 u_j^{n+1} = u_j^{n-1} + \lambda(u_{j+1}^n - u_j^n)
\]

where \( \lambda := k/h \). For \( \lambda = 0.9 \), \( u = 0 \) at the right hand boundary and initial data exact, consider the two possible left-hand boundary conditions: a) \( u_0^{n+1} = u_1^n \) and b) \( u_N^{n+1} = u_1^{n+1} \). Discuss which is likely to be stable and which unstable.

19. **Elliptic PDEs.** Consider the 1D BVP \( u_{xx} = f(x) \) with \( u(0) = 0 \) and \( u(1) = 1 \). Write down the finite set of equations which \( u_j \) must solve if a uniform grid with \( h = 1/N \) is used to discretise the equation and centred differences are used. Show that the discretized system admits the exact solution when \( f(x) := 2 \) and therefore solves the problem exactly for all \( N \). Explain why and discuss for what other choices of \( f(x) \) this also holds true. In 2D, so \( u_{xx} + u_{yy} = f(x,y) \), which \( f(x,y) \) will also give this result?

20. **Conjugate Gradient Method.** Solve the linear system

\[
\begin{pmatrix}
3 & 0 & 1 \\
0 & 2 & 0 \\
1 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
x
\end{pmatrix}
=
\begin{pmatrix}
2 \\
0 \\
0
\end{pmatrix}
\]

using the Conjugate Gradient Method. Using the characteristic polynomial of \( A \)

\[
A^3 - 6A^2 + 10A - 4I = 0,
\]

write down the answer as a sum of matrix multiplications involving \( A \) and check that this coincides with your conjugate gradient result.

21. **Fourier Spectral Methods.** Consider a function \( u(x) \) specified over a uniform grid of \( N + 1 \) pts such that \( u_j := u(x_j) \) where \( x_j := 2\pi j/N \) for \( j = 0,1,2,...N \) and the function is periodic \( (u_0 = u_N) \). The discrete Fourier Transform is defined as

\[
\hat{u}_k := \frac{1}{N} \sum_{j=1}^{N} u_j e^{-ikx_j}
\]

for \(-K \leq k \leq K \) and \( N = 2K+1 \). Derive an expression for the inverse discrete Fourier Transform.
22. Fourier Spectral Methods. Consider the heat equation \( u_t = u_{xx} \) over \([0, 2\pi]\) and initial condition
\[
u(x, 0) = \begin{cases} 
0 & x \neq \pi, \\
1 & x = \pi.
\end{cases}
\]
Formally we could adopt the boundary conditions \( u_x(0, t) = u_x(2\pi, t) = 0 \) or \( u(0, t) = u(2\pi, t) = 0 \) to complete the problem specification but given the (severely) localised initial conditions and short enough times, these are not that important. Also we don’t expect the solution to be \( 2\pi \)-periodic for subsequent times but it will so close to zero at the ends that it can be regarded as periodic in practice. So solve this problem using a Fourier Spectral method based on the uniform grid \( x_j := \frac{2\pi j}{N} \) for \( j = 0, 1, 2, \ldots, N \) to find
\[
u_j(t) = \frac{1}{N} \sum_{k=-K}^{K} e^{ik(x_j-\pi)-k^2t} \quad (*)
\]
where \( N = 2K + 1 \) (HINT: to make this manageable adopt the simplification that one of the grid points is precisely at \( \pi \)). Confirm this satisfies the heat equation (to get the i.c. to work will require reversing the simplification!). Note also that the sum \((*)\) at \( t = 0 \) does not show any spectral drop off. Try a smoother initial condition and convince yourself that the initial sum will then show this drop off.

23. Fourier Spectral Methods. Consider the variable coefficient wave equation
\[
u_t + c(x)u_x = 0, \quad c(x) := 0.2 + \sin^2(x - 1)
\]
for \( x \in [0, 2\pi], t > 0 \) with periodic boundary conditions and \( u(x, 0) = \exp(-100(x - 1)^2) \). As in previous question, this function is not mathematically periodic, but it is so close to zero at the ends of the interval that it can be regarded as periodic in practice. The following program uses the Leapfrog formula for the time derivative and spectral differentiation for the spatial derivative.

```matlab
% Fourier Spectral Method
% Grid, variable coefficient, and initial data
N=128;h=2*pi/N,x=h*(1:N),t=0,dt=h/4; ii=sqrt(-1);
c=0.2+sin(x-1).^2;
% To obtain v_1 to initiate Leapfrog we extrapolate backward in time
% assuming c is the constant wave speed of 0.2
v=exp(-100*(x-1).^2);vold=exp(-100*(x-0.2*dt-1).^2);
% Time-stepping by leap frog formula
tmax=8; tplot=0.15; clf, drawnow
plotgap=round(tplot/dt);dt=tplot/plotgap;
nplots=round(tmax/tplot);
data=[v;zeros(nplots,N)];tdata=t;
for j=1:nplots
    for n=1:plotgap
```
Figure 1: The solution to $Q_{23}$.

```matlab
t=t+dt;
v_hat=fft(v);
w_hat=ii*[0:N/2-1 0 -N/2+1:-1].*v_hat;
w=real(ifft(w_hat));
vnew=vold-2*dt*c.*w; vold=v;v=vnew;
end
data(j+1,:)=v;tdata=[tdata;t];
end
waterfall(x,tdata,data),view(10,70),colormap([0 0 0])
axis([0 2*pi 0 tmax 0 5]),ylabel t, zlabel u, grid off
```

(from “Spectral Methods in Matlab” Trefethen [4] p26). The result is a wave propagating at variable speed: see Figure 1.

24. Fourier Spectral Methods. Let $u(x) = \cos(mx)$ for some integer $m$. Calculate $uu_x$ by taking a discrete Fourier Transform

$$(\hat{uu}_x)_k := \sum_{p,q=-K}^{K} \hat{u}_p(\hat{u}_x)_q = \sum_{p,q=-K}^{K} iq \hat{u}_p \hat{u}_q,$$

simplify this convolution and then take the inverse Fourier Transform. Confirm your result by evaluating the product directly.

Spectral codes actually work in the reverse direction! One works in spectral space with $\hat{u}_k$ and one needs $(\hat{u}u_x)_k$. The approach is then to inverse transform $\hat{u}_k$ and $ik\hat{u}_k$ back to physical space.
to get $u$ and $u_x$ (respectively), evaluate $uu_x$ by (simple) multiplication and then Fourier transform this back to spectral space avoiding a costly convolution computation. Run through this.

25. **Chebyshev Polynomials.** Show that

(a) \( T_{2n}(x) = T_n(2x^2 - 1) = 2T_n(x)^2 - 1, \)

(b) \( T_{n+1}(x) = 2xT_n(x) - T_n(x), \)

(c) \( \frac{dT_n(x)}{dx} = \frac{n \sin n\theta}{\sin \theta} \quad \text{where } x = \cos \theta, \)

(d) \( \frac{d^2T_n(x)}{dx^2} = \frac{n \sin n\theta \cos \theta}{\sin^3 \theta} - \frac{n^2 \cos n\theta}{\sin^2 \theta} \quad \text{where } x = \cos \theta. \)

26. **Chebyshev Spectral Methods.** Show that the set of Chebyshev polynomials \( \{T_n(x) : n \in \{0, N\}\} \) is complete over \([-1, 1]\) by considering a general function \( f(x) \) and defining \( \theta := \cos^{-1} x. \) Formally, the interval \( x \in [-1, 1] \) maps to \( \theta \in [0, \pi] \) but \( f(\cos \theta) \) can be extended over \([0, 2\pi]\) by noticing a symmetry. With this symmetry, show that a subset of the complete Fourier set \( \{1, \cos n\theta, \sin n\theta : n \in \mathbb{N}\} \) over \([0, 2\pi]\) is then sufficient to represent any such function and relate this reduced set back to the set of Chebyshev polynomials.

27. **Chebyshev Spectral Methods.** Consider the eigenvalue problem

\[ u_{xx} + \lambda^2 u = 0 \]

over \([-1, 1]\) with \( u(\pm 1) = 0 \) where \( \lambda \) is the eigenvalue. Solve this problem using Chebyshev spectral methods adopting the following different strategies.

(a) Use a Tau method.

(b) Use a collocation method explicitly imposing the b.c.s.

(c) Use a collocation method implicitly imposing the b.c.s (i.e. build the b.c.s into the spectral functions: e.g. use \( \phi_n := T_{n+2}(x) - T_n(x) \); or \( \phi_n := (1 - x^2)T_n(x) \); or \( \phi_n := T_n(x) - 1 \) (n even) and \( \phi_n := T_n(x) - T_1(x) \) (n odd)).

(see Q25 for derivative expressions for Chebyshev polynomials).