Case Study # 4: Linear 1D Transport Equation

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1 Problem Description

The transport of various scalar quantities (e.g species mass fraction, temperature) in flows can be modeled using a linear convection-diffusion equation (presented here in a 1-D form),

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = D \frac{\partial \phi^2}{\partial x^2} \tag{1}$$

 ϕ is the transported scalar, u and D are known parameters (flow velocity and diffusion coefficient respectively). The purpose of this case study is to investigate the behavior of various numerical solutions of this equation.

This case study focuses on the solution of the 1-D linear transport equation (above) for $x \in [0,L]$ and $t \in [0,\tau]$ (where $\tau = 1/k^2D$) subject to periodic boundary conditions and the following initial condition

$$\phi(x,0) = \sin(kx),\tag{2}$$

with $k = 2\pi/L$ and L = 1 m. The convection velocity is u = 0.2 m/s, and the diffusion coefficient is D = 0.005 m²/s.

This problem has an analytical solution [1],

$$\Phi(x,t) = \exp(-k^2Dt)\sin[k(x-ut)]. \tag{3}$$

Numerical solutions of this problem were created using the following schemes:

- 1. FTCS (Explicit) Forward-Time and central differencing for both the convective flux and the diffusive flux.
- 2. Upwind Finite Volume method: Explicit (forward Euler), with the convective flux treated using the basic upwind method and the diffusive flux treated using central differencing.
- 3. Trapezoidal (AKA Crank-Nicholson).
- 4. QUICK Finite Volume method: Explicit, with the convective flux treated using the QUICK method and the diffusive flux treated using central differencing.

The following cases are considered:

$$(C,s) \in \{(0.1,0.25), (0.5,0.25), (2,0.25), (0.5,0.5), (0.5,1)\}$$

where $C = u\Delta t/\Delta x$ and $s = D\Delta t/\Delta x^2$. A uniform mesh for all solvers and cases. The stability and accuracy of these schemes was investigated.

2 Numerical Solution Approach

Four schemes were developed to deal with the five considered cases. These are an explicit FTCS scheme, an upwind finite volume scheme, an implicit trapezoidal scheme, and a QUICK finite volume scheme. Each case makes use of C and s to to compute the spatial ($\Delta x = CD/us$) and temporal ($\Delta t = C\Delta x/u$) discretizations.

2.1 FTCS Scheme

The first scheme involves using forward-time and central differencing (FTCS) for both the convective flux and the diffusive flux and yields second-order convergence in space and first-order convergence in time. In order to implement this method, the domain of the problem must be discretized. This method calculates the state of the system at a later time from the state of the system at the current time, and is thus an explicit method. For the 1-D transport equation on a uniform grid, the state ϕ at grid point i and timestep f can be calculated by the following equation,

$$\phi_i^f = \left(1 - \frac{2D\Delta t}{\Delta x^2}\right) \phi_i^{f-1} + \left(\frac{D\Delta t}{\Delta x^2} + \frac{u\Delta t}{2\Delta x}\right) \phi_{i-1}^{f-1} + \left(\frac{D\Delta t}{\Delta x^2} - \frac{u\Delta t}{2\Delta x}\right) \phi_{i+1}^{f-1}.$$
(4)

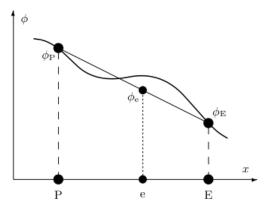


Fig. 1: The 1-D FTCS scheme interpolates between the two nearby grid points

This scheme is numerically stable as long as the following conditions are satisfied:

$$C \le \sqrt{2su}$$
 and $s \le \frac{1}{2}$. (5)

2.2 Upwind Scheme

The second scheme is an explicit upwind finite volume method. For this method the convective flux is treated using the basic upwind method and the diffusive flux treated using central differencing. This is a second-order scheme which uses a three point backward difference, as described below

$$\phi_{i}^{f} = \left(\frac{D\Delta t}{\Delta x^{2}}\right) \left[\phi_{i+1}^{f-1} - 2\phi_{i}^{f-1} + \phi_{i-1}^{f-1}\right] - \left(\frac{u\Delta t}{2\Delta x}\right) \left[3\phi_{i}^{f-1} - 4\phi_{i-1}^{f-1} + \phi_{i-2}^{f-1}\right] + \phi_{i}^{f-1}.$$
(6)

The upwind method is more stable than the FTCS scheme. Unlike the FTCS scheme, the stability of the Upwind scheme does not depend on *u*. This scheme is numerically stable as long as the following condition is satisfied:

$$C + 2s \le 1. \tag{7}$$

2.3 Trapezoidal (Crank-Nicholson) Scheme

$$\begin{bmatrix} b & c & & a \\ a & b & c & & \\ a & b & \ddots & & \\ b & c & & \ddots & c \\ c & & a & b & \\ \end{bmatrix} \begin{bmatrix} \phi_1^f \\ \phi_2^f \\ \phi_3^f \end{bmatrix} = \begin{bmatrix} RHS_1^f \\ RHS_2^f \\ RHS_3^f \\ \vdots \\ RHS_i^f \end{bmatrix}, \tag{8}$$

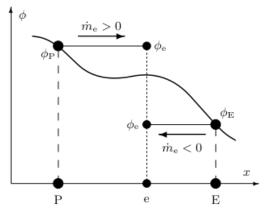


Fig. 2: Upwind scheme's interpolation for the diffusive flux

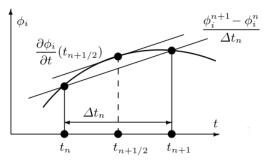


Fig. 3: Trapezoidal scheme

where c = A + B, b = 1 + 2A, and a = A - B, where

$$A = -\frac{D\Delta t}{2\Delta r^2} \text{ and } B = \frac{u\Delta t}{4\Delta r},$$
 (9)

and

$$RHS_{i}^{f} = A(\phi_{i+1}^{f-1} - 2\phi_{i}^{f-1} + \phi_{i-1}^{f-1}) - B(\phi_{i+1}^{f-1} - \phi_{i-1}^{f-1}) + \dots$$

$$\phi_{i}^{f-1}$$

$$(10)$$

The trapezoidal scheme is always stable.

2.4 QUICK Scheme

$$\begin{aligned} \phi_{i}^{f} &= \left(\frac{D\Delta t}{\Delta x^{2}}\right) \left[\phi_{i+1}^{f-1} - 2\phi_{i}^{f-1} + \phi_{i-1}^{f-1}\right] - \\ &\left(\frac{u\Delta t}{8\Delta x}\right) \left[3\phi_{i+1}^{f-1} + 3\phi_{i}^{f-1} + \phi_{i-2}^{f-1} - 7\phi_{i-1}^{f-1}\right] + \\ &\phi_{i}^{f-1} \end{aligned}$$

$$(11)$$

$$C \le \min(2 - 4s, \sqrt{2s}) \tag{12}$$

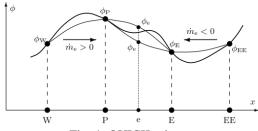


Fig. 4: QUICK scheme

3 Results Discussion

For the results below, cases 1, 2, 3, 4, 5 refer to (C,s)=(0.1,0.25),(0.5,0.25),(2,0.25),(0.5,0.5),(0.5,1), respectively. The stability for each scheme was investigated for each case. The stability criteria for the FTCS, Upwind, and QUICK schemes can be found as Equations 5, 7, and 12. For the cases considered, FTCS was least stable, the Upwind and QUICK schemes were equally stable, and the Trapezoidal scheme is always stable. For the full results, see Table 1.

Case	FTCS	Upwind	Trap	QUICK
1	True	True	True	True
2	False	True	True	True
3	False	False	True	False
4	False	False	True	False
5	False	False	True	False

Table 1: Stability results for each case and method

The computational result for the 1-D linear convectiondiffusion equation can be compared to the analytical result above, Equation 3. The Root Mean Square error,

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} [\phi_i - \phi_i^*]^2},$$
 (13)

and the Normalized Root Mean Square error,

$$NRMS = \frac{RMSE}{max(\phi^*) - min(\phi^*)},$$
 (14)

can be calculated. Here ϕ_i is the computational result for the the transported scalar for each point on the 1-D domain, ϕ_i^* is the analytical solution, and N is the number of points on the 1-D domain. The *NRMS* for each case is expressed as a percentage, where lower values indicate a result closer to the analytic solution.

Case	FTCS	Upwind	Trap	QUICK
1	7.23E-3	2.20E-2	2.42E-2	2.45E-2
2	2.23E-1	2.34E+10	1.30E-1	2.59E-1
3	8.26E+0	1.18E+2	7.72E-1	9.40E+0
4	1.06E-1	4.22E+36	4.56E-2	8.73E+11
5	1.10E+61	8.22E+110	2.14E-2	4.70E+85

Table 2: NRMS results for each case and method

4 Conclusion

References

- [1] Tannehill, J. C., Anderson, D. A., and Pletcher, R. C., 1997. *Computational Fluid Mechanics and Heat Transfer*, 2nd ed. Taylor & Francis.
- [2] Hogarth, W., Noye, B., Stagnitti, J., Parlange, J., and Bolt, G., 1990. "A comparative study of finite difference methods for solving the one-dimensional transport equation with an initial-boundary value discontinuity". *Computers & Mathematics with Applications*, **20**(11), pp. 67–82.
- [3] Chen, Y., and Falconer, R. A., 1992. "Advection-diffusion modelling using the modified quick scheme". *International journal for numerical methods in fluids*, **15**(10), pp. 1171–1196.
- [4] Tryggvason, G., 2013. The advection-diffusion equation. http://www3.nd.edu/ gtryggva/CFD-Course/.

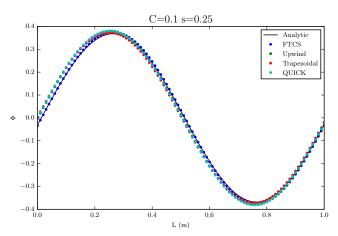


Fig. 5: Results of first case

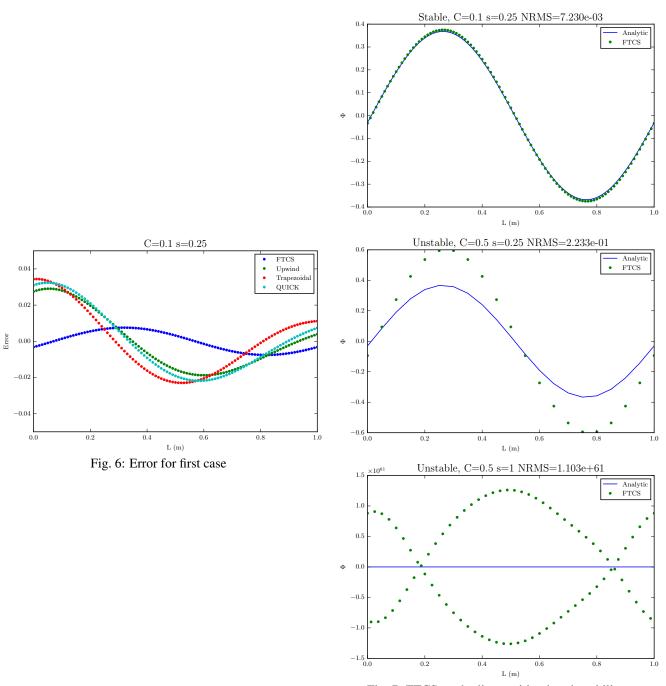


Fig. 7: FTCS method's transition into instability

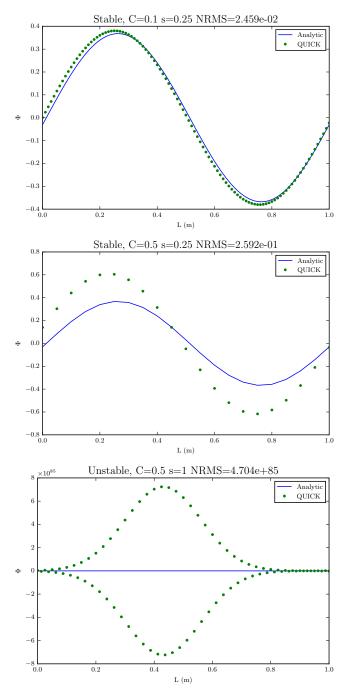


Fig. 8: QUICK method's transition into instability

Appendix A: Python Code

```
| from PrettyPlots import *
  import numpy as np
  import matplotlib.pyplot as plt
  from scipy import log10
  from scipy.optimize import curve_fit
  import scipy.sparse as sparse
  import os
10 class Config(object):
    def __init__(self, C, s):
          # Import parameters
13
          self.C = C
          self.s = s
14
15
         # Problem constants
16
         self.L = 1.
                                         # m
17
         self.D = 0.005
18
                                         # m^2/s
         self.u = 0.2
19
                                         # m/s
          self.k = 2 * np.pi / self.L # m^-1
20
          self.tau = 1 / (self.k ** 2 * self.D)
22
23
          # Set-up Mesh and Calculate time-step
          self.dx = self.C * self.D / (self.u * self.s)
24
          self.dt = self.C * self.dx / self.u
          self.x = np.append(np.arange(0, self.L, self.dx), self.L)
27
  def Analytic(c):
29
      k, D, u, tau, x = c.k, c.D, c.u, c.tau, c.x
30
31
      N = len(x)
32
      Phi = np.array(x)
34
      for i in range(0, N):
35
36
         Phi[i] = np.exp(-k ** 2 * D * tau) * np.sin(k * (x[i] - u * tau))
      return np.array(Phi)
38
39
  def FTCS(Phi, c):
41
40
      FTCS (Explicit) - Forward-Time and central differencing for both the
43
      convective flux and the diffusive flux.
45
46
      D, dt, dx, u, tau = c.D, c.dt, c.dx, c.u, c.tau
47
48
      N = len(Phi)
49
50
      Phi = np.array(Phi)
      Phi_old = np.array(Phi)
52
      t = 0
53
      while t < tau:</pre>
54
          for i in range(1, N - 1):
55
              Phi[i] = ((1 - 2 * D * dt / dx ** 2) * Phi_old[i] +
56
                         (D * dt / dx ** 2 + u * dt / (2 * dx)) * Phi_old[i - 1] +
57
                         (D * dt / dx ** 2 - u * dt / (2 * dx)) * Phi_old[i + 1])
58
59
          # Enforce our periodic boundary condition
60
          Phi[-1] = ((1 - 2 * D * dt / dx ** 2) * Phi_old[-1] +
61
                      (D * dt / dx ** 2 + u * dt / (2 * dx)) * Phi_old[-2] +
62
                      (D * dt / dx ** 2 - u * dt / (2 * dx)) * Phi_old[1])
63
          Phi[0] = Phi[-1]
64
65
          Phi_old = np.array(Phi)
66
          t += dt
```

```
69
                    return np.array(Phi_old)
  70
        def Upwind(Phi, c):
                     Upwind-Finite Volume method: Explicit (forward Euler), with the convective
                     flux treated using the basic upwind method and the diffusive flux treated
                    using central differencing.
  76
                    111
  78
                    D, dt, dx, u, tau = c.D, c.dt, c.dx, c.u, c.tau
  79
  80
                    N = len(Phi)
  81
                    Phi = np.array(Phi)
  82
                    Phi_old = np.array(Phi)
  83
                    t = 0
  8.5
                    while t <= tau:</pre>
  86
                                Phi[0] = (D * dt / dx ** 2 * (Phi_old[1] - 2 * Phi_old[0] + Phi_old[-1]) -
  87
  88
                                                              u * dt / (2 * dx) * (3 * Phi_old[0] - 4 * Phi_old[-1] + Phi_old[-2]) +
                                                              Phi_old[0])
  89
  90
                                Phi[1] = (D * dt / dx ** 2 * (Phi_old[2] - 2 * Phi_old[1] + Phi_old[0]) - (Phi_old[1] + Phi_old[1]) - (Phi_old[1
  91
                                                               u * dt / (2 * dx) * (3 * Phi_old[1] - 4 * Phi_old[0] + Phi_old[-1]) +
  92
  93
                                                              Phi_old[1])
  94
                                for i in range (2, N - 1):
  95
                                             Phi[i] = (D * dt / dx ** 2 * (Phi_old[i + 1] - 2 * Phi_old[i] + Phi_old[i - 1]) - (Phi_old[i + 1] + Phi_old[i] + (Phi_old[i - 1]) - (Phi_old[i] + Phi_old[i] + (Phi_old[i] + (Phi_old[i] + Phi_old[i] + (Phi_old[i] + (Phioold[i] + (Ph
  96
  97
                                                                           u * dt / (2 * dx) * (3 * Phi_old[i] - 4 * Phi_old[i - 1] + Phi_old[i - 2]) +
  98
                                                                           Phi_old[i])
 99
                                Phi[-1] = (D * dt / dx ** 2 * (Phi_old[0] - 2 * Phi_old[-1] + Phi_old[-2]) -
100
                                                                  u * dt / (2 * dx) * (3 * Phi_old[-1] - 4 * Phi_old[-2] + Phi_old[-3]) +
101
                                                                  Phi_old[-1])
102
103
                              Phi_old = np.array(Phi)
104
105
                                t += dt
106
                    return np.array(Phi_old)
107
108
109
         def Trapezoidal(Phi, c):
110
                    D, dt, dx, u, tau = c.D, c.dt, c.dx, c.u, c.tau
111
                    N = len(Phi)
114
                    Phi = np.array(Phi)
                    Phi_old = np.array(Phi)
115
116
                     # Create Coefficient Matrix
                    upper = [-(dt * D) / (2 * dx ** 2) + dt * u / (4 * dx) for _ in range(0, N)]
118
                     main = [1 + (dt * D / (dx ** 2)) for _ in range(0, N)]
                    lower = [-(dt * D) / (2 * dx ** 2) - dt * u / (4 * dx) for _ in range(0, N)]
120
                    data = lower, main, upper
122
                    diags = np.array([-1, 0, 1])
                    matrix = sparse.spdiags(data, diags, N, N).todense()
124
125
                    # Set values for cyclic boundary conditions
126
                    matrix[0, N-1] = -(dt * D) / (2 * dx ** 2) - dt * u / (4 * dx)
                    matrix[N - 1, 0] = -(dt * D) / (2 * dx ** 2) + dt * u / (4 * dx)
128
120
                    # create blank b array
130
131
                    b = np.array(Phi_old)
133
                    t = 0
                    while t <= tau:</pre>
134
                                # Enforce our periodic boundary condition
                                b[0] = ((dt * D / (2 * dx ** 2)) * (Phi_old[1] - 2 * Phi_old[0] + Phi_old[-1]) -
136
```

```
(u * dt / (4 * dx)) * (Phi_old[1] - Phi_old[-1]) +
138
                                                                           Phi_old[0])
139
                                          for i in range(1, N - 1):
140
                                                          b[i] = ((dt * D / (2 * dx ** 2)) * (Phi_old[i + 1] - 2 * Phi_old[i] + Phi_old[i - 1]) - (dt * D / (2 * dx ** 2)) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2)) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) * (Phi_old[i + 1] + (dt * D / (2 * dx ** 2))) 
141
                                                                                            (u * dt / (4 * dx)) * (Phi_old[i + 1] - Phi_old[i - 1]) +
142
143
                                                                                           Phi_old[i])
                                            # Enforce our periodic boundary condition
144
                                          b[-1] = ((dt * D / (2 * dx ** 2)) * (Phi_old[0] - 2 * Phi_old[-1] + Phi_old[-2]) -
146
147
                                                                                (u * dt / (4 * dx)) * (Phi_old[0] - Phi_old[-2]) +
                                                                               Phi_old[-1])
148
149
                                           # Solve matrix
150
                                          Phi = np.linalq.solve(matrix, b)
                                          Phi_old = np.array(Phi)
153
                                          t += dt
156
                          return np.array(Phi_old)
157
158
          def QUICK(Phi, c):
                          D, dt, dx, u, tau = c.D, c.dt, c.dx, c.u, c.tau
160
161
                          N = len(Phi)
162
                          Phi = np.array(Phi)
163
                          Phi_old = np.array(Phi)
164
165
                          t = 0
166
                          while t <= tau:</pre>
167
                                          Phi[0] = (dt * D / dx ** 2 * (Phi_old[1] - 2 * Phi_old[0] + Phi_old[N - 1]) -
168
                                                                                    dt * u / (8 * dx) * (3 * Phi_old[1] + Phi_old[-2] - 7 * Phi_old[N - 1] + 3 * Phi_old[0]) +
169
                                                                                   Phi_old[0])
170
                                          Phi[1] = (dt * D / dx ** 2 * (Phi_old[2] - 2 * Phi_old[1] + Phi_old[0]) -
171
                                                                                   dt * u / (8 * dx) * (3 * Phi_old[2] + Phi_old[N - 1] - 7 * Phi_old[0] + 3 * Phi_old[1]) +
                                                                                   Phi_old[1])
174
175
                                          for i in range (2, N - 1):
                                                          Phi[i] = (dt * D / dx ** 2 * (Phi_old[i + 1] - 2 * Phi_old[i] + Phi_old[i - 1]) - 2 * Phi_old[i] + Phi_old[
176
                                                                                                    dt * u / (8 * dx) * (3 * Phi_old[i + 1] + Phi_old[i - 2] - 7 * Phi_old[i - 1] + 3 * Phi_old[i];
178
                                                                                                    Phi_old[i])
179
                                          Phi[-1] = (dt * D / dx ** 2 * (Phi_old[0] - 2 * Phi_old[-1] + Phi_old[-2]) - Phi_old[-2]) - Phi_old[-2] + Phi_old[-2]) - Phi_old[-2] + Phi_o
180
                                                                                       dt * u / (8 * dx) * (3 * Phi_old[0] + Phi_old[-3] - 7 * Phi_old[-2] + 3 * Phi_old[-1]) +
181
                                                                                        Phi_old[-1])
182
183
184
                                            # Increment
                                          Phi_old = np.array(Phi)
184
                                          t += dt
186
187
188
                           return np.array(Phi_old)
189
190
          def save_figure(x, analytic, solution, title, stable):
191
                          plt.figure(figsize=fig_dims)
192
193
                          plt.plot(x, analytic, label='Analytic')
194
                          plt.plot(x, solution, '.', label=title.split(' ')[0])
195
196
197
                           # Calculate NRMS for this solution
                          err = solution - analytic
198
                          NRMS = np.sqrt(np.mean(np.square(err)))/(max(analytic) - min(analytic))
199
200
                          plt.ylabel('$\Phi$')
201
202
                          plt.xlabel('L (m)')
203
                           if stable:
204
                                          stability = 'Stable, '
```

```
else:
206
207
           stability = 'Unstable, '
208
       plt.title(stability +
209
                  'C=' + title.split(' ')[1] +
                  ' s=' + title.split(' ')[2] +
                  ' NRMS={0:.3e}'.format(NRMS))
212
213
       plt.legend(loc='best')
       # Save plots
216
       save_name = title + '.pdf'
217
          os.mkdir('figures')
218
       except Exception:
219
          pass
220
221
       plt.savefig('figures/' + save_name, bbox_inches='tight')
       plt.close()
226
   def save_state(x, analytic, solutions, state):
       plt.figure(figsize=fig_dims)
       plt.plot(x, analytic, 'k', label='Analytic')
229
       for solution in solutions:
230
           plt.plot(x, solution[0], '.', label=solution[1])
       plt.ylabel('$\Phi$')
      plt.xlabel('L (m)')
234
235
       title = 'C=' + state.split(' ')[0] + ' s=' + state.split(' ')[1]
236
       plt.title(title)
       plt.legend(loc='best')
238
240
       # Save plots
       save_name = title + '.pdf'
241
242
          os.mkdir('figures')
243
244
       except Exception:
249
          pass
246
       plt.savefig('figures/' + save_name, bbox_inches='tight')
247
       plt.close()
249
2.50
251
   def save_state_error(x, analytic, solutions, state):
       plt.figure(figsize=fig_dims)
253
       for solution in solutions:
254
           Error = solution[0] - analytic
           plt.plot(x, Error, '.', label=solution[1])
256
       plt.ylabel('Error')
258
       plt.xlabel('L (m)')
       plt.ylim([-0.05, 0.05])
260
261
       title = 'C=' + state.split(' ')[0] + ' s=' + state.split(' ')[1]
262
263
       plt.title(title)
       plt.legend(loc='best')
264
265
       # Save plots
       save_name = 'Error ' + title + '.pdf'
267
268
          os.mkdir('figures')
269
       except Exception:
270
271
       plt.savefig('figures/' + save_name, bbox_inches='tight')
       plt.close()
```

```
276
   def plot_order(x, t, RMS):
       fig = plt.figure(figsize=fig_dims)
278
       RMS, title = RMS[0], RMS[1]
280
281
       # Find effective order of accuracy
282
       order_accuracy_x = effective_order(x, RMS)
283
       order_accuracy_t = effective_order(t, RMS)
2.84
       # print(title, 'x order: ', order_accuracy_x, 't order: ', order_accuracy_t)
285
287
       # Show effect of dx on RMS
       fig.add_subplot(2, 1, 1)
288
       plt.plot(x, RMS, '.')
289
       plt.title('dx vs RMS, effective order {0:1.2f}'.format(order_accuracy_x))
290
       plt.xscale('log')
       plt.yscale('log')
292
       plt.xlabel('dx')
293
294
       plt.ylabel('NRMS')
295
       fig.subplots_adjust(hspace=.35)
296
       # Show effect of dt on RMS
297
       fig.add_subplot(2, 1, 2)
298
       plt.plot(t, RMS, '.')
300
       plt.title('dt vs RMS, effective order {0:1.2f}'.format(order_accuracy_t))
       plt.xscale('log')
301
       plt.yscale('log')
302
       plt.xlabel('dt')
303
304
       plt.ylabel('NRMS')
305
       # Slap the method name on
306
       plt.suptitle(title)
307
308
309
       # Save plots
       save_name = 'Order ' + title + '.pdf'
311
          os.mkdir('figures')
312
313
       except Exception:
314
          pass
315
       plt.savefig('figures/' + save_name, bbox_inches='tight')
       plt.close()
317
320
  def stability(c):
321
       C, s, u = c.C, c.s, c.u
       FTCS = C <= np.sqrt(2 * s * u) and s <= 0.5
       Upwind = C + 2*s \le 1
324
       Trapezoidal = True
325
326
       QUICK = C \le \min(2 - 4 * s, \operatorname{np.sqrt}(2 * s))
       # print('C = ', C, ' s = ', s)
       # print('FTCS: ' + str(FTCS))
329
       # print('Upwind: ' + str(Upwind))
330
       # print('Trapezoidal: ' + str(Trapezoidal))
       # print('QUICK: ' + str(QUICK))
       return [FTCS, Upwind, Trapezoidal, QUICK]
334
335
336
   def linear_fit(x, a, b):
       ""Define our (line) fitting function"
338
339
       return a + b * x
340
341
342 def effective_order(x, y):
       ""Find slope of log log plot to find our effective order of accuracy"
```

```
344
345
       logx = log10(x)
       logy = log10(y)
       out = curve_fit(linear_fit, logx, logy)
347
348
       return out[0][1]
349
350
351
  def calc_stability(C, s, solver):
352
       results = []
353
354
       for C_i, s_i in zip(C, s):
355
           out = generate_solutions(C_i, s_i, find_order=True)
356
           results.append(out)
357
       # Sort and convert
358
       results.sort(key=lambda x: x[0])
359
360
       results = np.array(results)
361
       # Pull out data
362
363
       x = results[:, 0]
364
       t = results[:, 1]
       RMS_FTCS = results[:, 2]
365
       RMS_Upwind = results[:, 3]
366
       RMS_Trapezoidal = results[:, 4]
367
       RMS_QUICK = results[:, 5]
368
369
       # Plot effective orders
       rms_list = [(RMS_FTCS, 'FTCS'),
                    (RMS_Upwind, 'Upwind'),
372
                    (RMS_Trapezoidal, 'Trapezoidal'),
373
                    (RMS_QUICK, 'QUICK')]
374
       for rms in rms_list:
376
377
           if rms[1] == solver:
378
                plot_order(x, t, rms)
380
  def generate_solutions(C, s, find_order=False):
381
382
      c = Config(C, s)
383
       # Spit out some stability information
384
       stable = stability(c)
385
       # Initial Condition with boundary conditions
387
       Phi_initial = np.sin(c.k * c.x)
388
389
390
       # Analytic Solution
       Phi_analytic = Analytic(c)
391
392
       # Explicit Solution
393
       Phi_ftcs = FTCS(Phi_initial, c)
394
       # Upwind Solution
396
       Phi_upwind = Upwind(Phi_initial, c)
397
398
       # Trapezoidal Solution
       Phi_trapezoidal = Trapezoidal(Phi_initial, c)
400
401
       # QUICK Solution
402
       Phi_quick = QUICK(Phi_initial, c)
403
404
       # Save group comparison
404
       solutions = [(Phi_ftcs, 'FTCS'),
406
                      (Phi_upwind, 'Upwind'),
407
408
                      (Phi_trapezoidal, 'Trapezoidal'),
                     (Phi_quick, 'QUICK')]
409
410
       if not find_order:
411
            # Save individual comparisons
412
```

```
save_figure(c.x, Phi_analytic, Phi_ftcs,
413
414
                        'FTCS ' + str(C) + ' ' + str(s), stable[0])
           save_figure(c.x, Phi_analytic, Phi_upwind,
415
416
                        'Upwind ' + str(C) + ' ' + str(s), stable[1])
           save_figure(c.x, Phi_analytic, Phi_trapezoidal,
417
                        'Trapezoidal ' + str(C) + ' ' + str(s), stable[2])
418
           save_figure(c.x, Phi_analytic, Phi_quick,
419
                        'QUICK ' + str(C) + ' ' + str(s), stable[3])
420
421
           # and group comparisons
420
423
           save_state(c.x, Phi_analytic, solutions, str(C) + ' ' + str(s))
           save_state_error(c.x, Phi_analytic, solutions, str(C) + ' ' + str(s))
424
425
      NRMS = []
426
       for solution in solutions:
427
           err = solution[0] - Phi_analytic
428
           NRMS.append(np.sqrt(np.mean(np.square(err)))/(max(Phi_analytic) - min(Phi_analytic)))
429
430
       return [c.dx, c.dt, NRMS[0], NRMS[1], NRMS[2], NRMS[3]]
431
432
433
  def main():
434
       # Cases
435
       C = [0.1,
                  0.5, 2, 0.5, 0.5]
436
       s = [0.25, 0.25, .25, 0.5,
437
438
       for C_i, s_i in zip(C, s):
          generate_solutions(C_i, s_i)
439
440
       # Stable values for each case to find effective order of methods
441
442
      C = [0.10, 0.50, 0.40, 0.35, 0.5]
       s = [0.25, 0.25, 0.25, 0.40, 0.5]
443
      calc_stability(C, s, 'FTCS')
444
445
      C = [0.1, 0.2, 0.3, 0.05, 0.1]
       s = [0.4, 0.3, 0.2, 0.15, 0.1]
447
      calc_stability(C, s, 'Upwind')
448
449
      C = [0.5, 0.6, 0.7, 0.8, 0.9]
450
       s = [0.25, 0.25, 0.25, 0.25, 0.25]
451
      calc_stability(C, s, 'Trapezoidal')
452
453
      C = [0.25, 0.4, 0.5, 0.6, 0.7]
454
       s = [0.25, 0.25, 0.25, 0.25, 0.25]
455
       calc_stability(C, s, 'QUICK')
456
457
458
  if __name__ == "__main__":
      main()
```

Listing 1: Code to create plots and solutions

```
import numpy as np
import matplotlib
matplotlib.use('TkAgg')

# Configure figures for production
WIDTH = 495.0  # the number latex spits out
FACTOR = 1.0  # the fraction of the width the figure should occupy
fig_width_pt = WIDTH * FACTOR

inches_per_pt = 1.0 / 72.27
golden_ratio = (np.sqrt(5) - 1.0) / 2.0  # because it looks good
fig_width_in = fig_width_pt * inches_per_pt # figure width in inches
fig_height_in = fig_width_in * golden_ratio # figure height in inches
fig_dims = [fig_width_in, fig_height_in] # fig dims as a list
```

Listing 2: Code to generate pretty plots