

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),

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = D \frac{\partial^2 \phi}{\partial x^2}, \quad (1)$$

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 $\tau = 1/k^2 D$) subject to periodic boundary conditions and the following initial condition

$$\phi(x, 0) = \sin(kx), \quad (2)$$

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],

$$\Phi(x, t) = \exp(-k^2 D t) \sin[k(x - ut)]. \quad (3)$$

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 investigate 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 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,

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

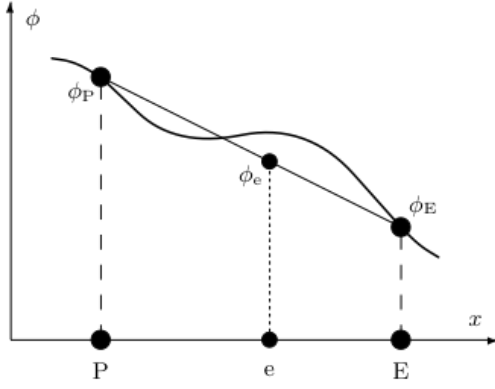


Fig. 1: The 1-D FTCS scheme interpolates between the two nearby grid points [1]

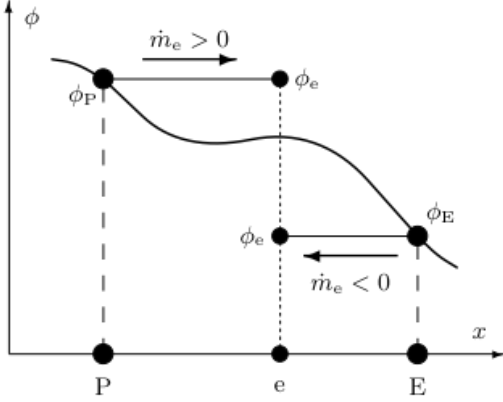


Fig. 2: Upwind scheme's interpolation for the diffusive flux [1]

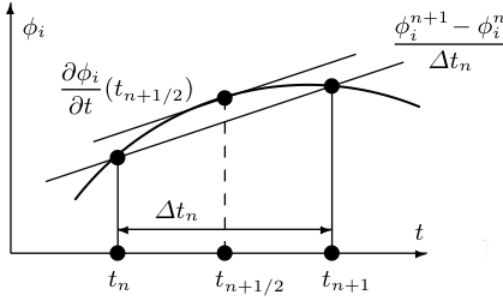


Fig. 3: Trapezoidal scheme's interpolation for the time derivative [1]

To impose the periodic boundary condition, the last node in the domain reaches around to the second node, while the first node is set equivalent to the last node. This scheme is numerically stable as long as the following conditions are satisfied:

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

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

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

The upwind method is more stable than the FTCS scheme, and unlike the FTCS scheme, the stability of the Upwind scheme does not depend on u . To impose the periodic boundary condition, the last node and the second node in the domain reach across the edge of the domain, while the first node is set equivalent to the last node. This scheme is numerically stable as long as the following condition is satisfied:

$$C + 2s \leq 1. \quad (7)$$

2.3 Trapezoidal (Crank-Nicholson) Scheme

The Trapezoidal scheme is a finite difference method which is implicit and unconditionally stable. This method is an equally weighted average of the explicit and implicit central difference solutions. As this is an implicit method, a system of algebraic equations must be solved to find values of the transported scalar for the next timestep. This problem requires the solution of a nearly tridiagonal matrix, with the exception of the top right and bottom left corners, which are set to impose the periodic boundary condition [2].

The following set of equations must be solved to advance the solution to the next timestep:

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

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

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

The right hand side of the equation is a linear combination of the solutions from the previous timestep,

$$\begin{aligned} RHS_i^f = & A(\phi_{i+1}^{f-1} - 2\phi_i^{f-1} + \phi_{i-1}^{f-1}) - \\ & B(\phi_{i+1}^{f-1} - \phi_{i-1}^{f-1}) + \\ & \phi_i^{f-1}. \end{aligned} \quad (10)$$

2.4 QUICK Scheme

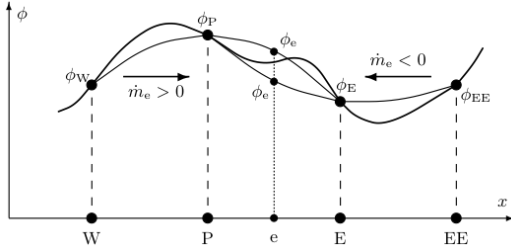


Fig. 4: The QUICK scheme interpolates between two quadratic equations [1]

The Quadratic Upstream Interpolation for Convective Kinematics (QUICK) method is an explicit method which uses three point upstream weighted quadratic interpolation for cell phase values (see Figure 4). Here the convective flux is treated using the QUICK method, while the diffusive flux treated using central differencing. This scheme is second-order accurate for the finite difference model [3]. This can be implemented with the following equation:

$$\begin{aligned} \phi_i^f = & \left(\frac{D\Delta t}{\Delta x^2} \right) \left[\phi_{i+1}^{f-1} - 2\phi_i^{f-1} + \phi_{i-1}^{f-1} \right] - \\ & \left(\frac{u\Delta t}{8\Delta x} \right) \left[3\phi_{i+1}^{f-1} + 3\phi_i^{f-1} + \phi_{i-2}^{f-1} - 7\phi_{i-1}^{f-1} \right] + \\ & \phi_i^{f-1} \end{aligned} \quad (11)$$

To impose the periodic boundary condition, the last node and the second node in the domain reach across the edge of the domain, while the first node is set equivalent to the last node. This scheme is numerically stable under the following condition:

$$C \leq \min(2 - 4s, \sqrt{2s}). \quad (12)$$

3 Results Discussion

3.1 Stability

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 [4]. For the cases considered, FTCS was least stable, the Upwind and QUICK schemes were effectively equally stable, and the Trapezoidal scheme is always stable. For the full results, see Table 1.

3.2 NRMS

The computational result for the 1-D linear convection-diffusion equation can be compared to the analytical result

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

Case	FTCS	Upwind	Trap	QUICK
1	7.23E-03	9.68E-03	2.42E-02	7.67E-03
2	2.23E-01	2.89E-01	1.30E-01	2.32E-01
3	8.26E+00	3.64E+01	7.72E-01	1.24E+01
4	1.06E-01	6.99E+22	4.56E-02	1.10E-01
5	1.10E+61	1.28E+97	2.14E-02	7.37E+71

Table 2: NRMS results for each case and method

above, Equation 3. The Root Mean Square error,

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

and the Normalized Root Mean Square error,

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

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. For the complete $NRMS$ results for each case and scheme, see Table 2.

The lowest $NRMS$ error is found by using the FTCS scheme under Case 1. Despite this, the FTCS case quickly blows up for Cases 3 and 5 due to numerical instability. The QUICK method performs similarly, with approximately the same error for all cases. The Trapezoidal method's unconditional stability leads to it performing best for all cases aside from Case 1.

The cases of large $NRMS$ arise from the loss of stability in the scheme. The effect of instability can be seen quite clearly in Figure 8. Making use of Equation 12 with values $C = 0.5$ and $s = 1$, for instance, one can see that

$$\begin{aligned} C &\leq \min(2 - 4s, \sqrt{2s}) \\ 0.5 &\leq \min(-2, \sqrt{2}) \\ 0.5 &\leq -2 \end{aligned} \quad (15)$$

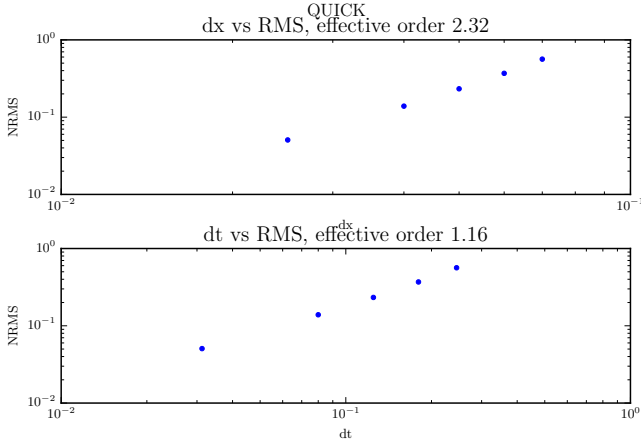


Fig. 5: Effective order of the QUICK method

Method	Δx	Δt
FTCS	2.06	1.06
Upwind	1.08	0.55
Trap	1.97	0.99
QUICK	2.32	1.16

Table 3: Effective order of each method for Δx and Δt

is false. This leads to the instability and resultant large NRMS of $4.70\text{E}+85$.

3.3 Effective Order

The effective order of each method was calculated by fitting the NRMS for cases within the stability region of each method. The effective order was found by fitting with a linear function against a log log plot of the NRMS versus the Δx and Δt , see Figure 5 for an example. The slope of the fit estimates the order of accuracy of the method. The effective orders of accuracy for the FTCS, Trapezoidal, and QUICK methods are approximately 2 for the spatial dimension and approximately 1 for the temporal dimension. The Upwind method is approximately first order accurate in the spatial dimension. For full results, see Table 3.

4 Conclusion

Only the first case led to stable solutions for each scheme. The results from this case can be seen in Figure 6. The error between each scheme's result and the analytic solution can be seen in Figure 7. This error shows that the three explicit methods can perform better than the implicit method for low CFL numbers, though for larger CFL numbers the opposite is true.

While the FTCS and QUICK schemes produced the lowest error in the majority of the considered cases, the unconditional stability of the Trapezoidal method makes it the more reliable method if the C and s values cannot be chosen freely.

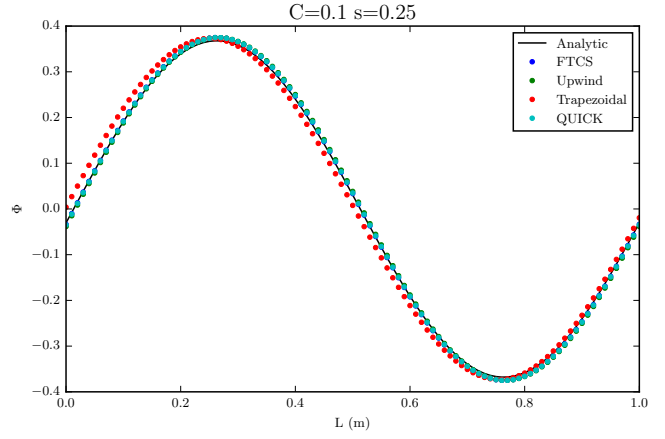


Fig. 6: Results of each scheme for Case 1

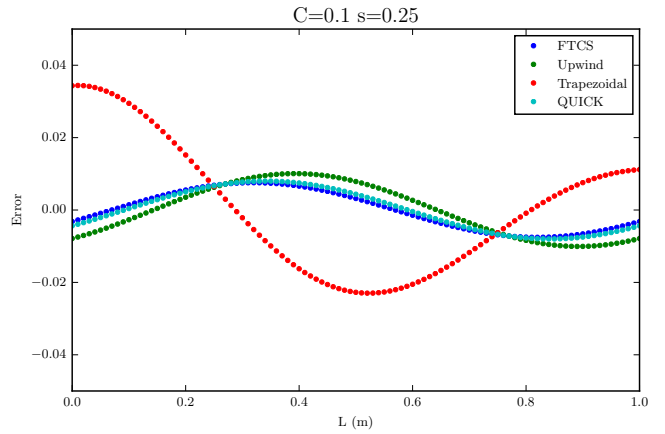


Fig. 7: Error for each scheme for Case 1

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/>.

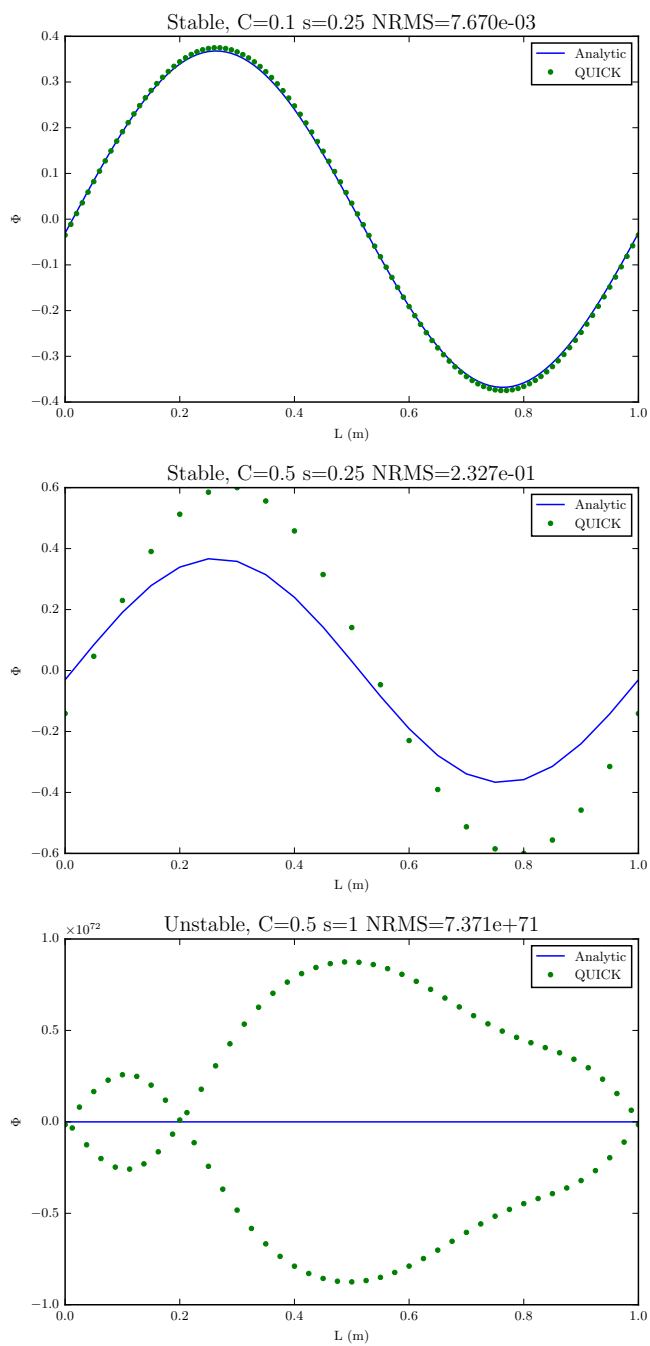


Fig. 8: QUICK method's transition into instability

Appendix A: Python Code

```
1 from PrettyPlots import *
2 import numpy as np
3 import matplotlib.pyplot as plt
4 from scipy import log10
5 from scipy.optimize import curve_fit
6 import scipy.sparse as sparse
7 import os
8
9
10 class Config(object):
11     def __init__(self, C, s):
12         # Import parameters
13         self.C = C
14         self.s = s
15
16         # Problem constants
17         self.L = 1. # m
18         self.D = 0.005 # m^2/s
19         self.u = 0.2 # m/s
20         self.k = 2 * np.pi / self.L # m^-1
21         self.tau = 1 / (self.k ** 2 * self.D)
22
23         # Set-up Mesh and Calculate time-step
24         self.dx = self.C * self.D / (self.u * self.s)
25         self.dt = self.C * self.dx / self.u
26         self.x = np.append(np.arange(0, self.L, self.dx), self.L)
27
28
29 def Analytic(c):
30     k, D, u, tau, x = c.k, c.D, c.u, c.tau, c.x
31
32     N = len(x)
33     Phi = np.array(x)
34
35     for i in range(0, N):
36         Phi[i] = np.exp(-k ** 2 * D * tau) * np.sin(k * (x[i] - u * tau))
37
38     return np.array(Phi)
39
40
41 def FTCS(Phi, c):
42     """
43     FTCS (Explicit) - Forward-Time and central differencing for both the
44     convective flux and the diffusive flux.
45     """
46
47     D, dt, dx, u, tau = c.D, c.dt, c.dx, c.u, c.tau
48
49     N = len(Phi)
50     Phi = np.array(Phi)
51     Phi_old = np.array(Phi)
52
53     A = D * dt / dx ** 2
54     B = u * dt / (2 * dx)
55
56     t = 0
57     while t < tau:
58         for i in range(1, N - 1):
59             Phi[i] = ((A + B) * Phi_old[i - 1] +
60                      (1 - 2 * A) * Phi_old[i] +
61                      (A - B) * Phi_old[i + 1])
62
63         # Enforce our periodic boundary condition
64         Phi[-1] = ((A + B) * Phi_old[-2] +
65                   (1 - 2 * A) * Phi_old[-1] +
66                   (A - B) * Phi_old[1])
67         Phi[0] = Phi[-1]
```

```

68     Phi_old = np.array(Phi)
69     t += dt
70
71
72     return np.array(Phi_old)
73
74
75 def Upwind(Phi, c):
76     """
77     Upwind-Finite Volume method: Explicit (forward Euler), with the convective
78     flux treated using the basic upwind method and the diffusive flux treated
79     using central differencing.
80     """
81
82     D, dt, dx, u, tau = c.D, c.dt, c.dx, c.u, c.tau
83
84     N = len(Phi)
85     Phi = np.array(Phi)
86     Phi_old = np.array(Phi)
87
88     A = D * dt / dx ** 2
89     B = u * dt / (2 * dx)
90
91     t = 0
92     while t <= tau:
93         for i in range(2, N - 1):
94             Phi[i] = (A * (Phi_old[i + 1] - 2 * Phi_old[i] + Phi_old[i - 1]) -
95                     B * (3 * Phi_old[i] - 4 * Phi_old[i - 1] + Phi_old[i - 2]) +
96                     Phi_old[i])
97
98             Phi[-1] = (A * (Phi_old[1] - 2 * Phi_old[-1] + Phi_old[-2]) -
99                     B * (3 * Phi_old[-1] - 4 * Phi_old[-2] + Phi_old[-3]) +
100                     Phi_old[-1])
101             Phi[0] = Phi[-1]
102             Phi[1] = (A * (Phi_old[2] - 2 * Phi_old[1] + Phi_old[-1]) -
103                     B * (3 * Phi_old[1] - 4 * Phi_old[-1] + Phi_old[-2]) +
104                     Phi_old[1])
105
106             Phi_old = np.array(Phi)
107             t += dt
108
109     return np.array(Phi_old)
110
111
112 def Trapezoidal(Phi, c):
113     D, dt, dx, u, tau = c.D, c.dt, c.dx, c.u, c.tau
114
115     N = len(Phi)
116     Phi = np.array(Phi)
117     Phi_old = np.array(Phi)
118
119     A = dt * D / (2 * dx**2)
120     B = dt * u / (4 * dx)
121
122     # Create Coefficient Matrix
123     lower = [-A - B for _ in range(0, N)]
124     main = [1 + 2 * A for _ in range(0, N)]
125     upper = [-A + B for _ in range(0, N)]
126
127     data = lower, main, upper
128     diags = np.array([-1, 0, 1])
129     matrix = sparse.spdiags(data, diags, N, N).todense()
130
131     # Set values for periodic boundary conditions
132     matrix[0, N - 1] = -A - B
133     matrix[N - 1, 0] = -A + B
134
135     # Initialize RHS
136     RHS = np.array(Phi_old)

```

```

137
138 t = 0
139 while t <= tau:
140     # Enforce our periodic boundary condition
141     RHS[0] = (A * (Phi_old[1] - 2 * Phi_old[0] + Phi_old[-1]) -
142              B * (Phi_old[1] - Phi_old[-1]) +
143              Phi_old[0])
144
145     for i in range(1, N - 1):
146         RHS[i] = (A * (Phi_old[i + 1] - 2 * Phi_old[i] + Phi_old[i - 1]) -
147                  B * (Phi_old[i + 1] - Phi_old[i - 1]) +
148                  Phi_old[i])
149
150     # Enforce our periodic boundary condition
151     RHS[-1] = (A * (Phi_old[0] - 2 * Phi_old[-1] + Phi_old[-2]) -
152               B * (Phi_old[0] - Phi_old[-2]) +
153               Phi_old[-1])
154
155     # Solve matrix
156     Phi = np.linalg.solve(matrix, RHS)
157
158     Phi_old = np.array(Phi)
159     t += dt
160
161     return np.array(Phi_old)
162
163
164 def QUICK(Phi, c):
165     D, dt, dx, u, tau = c.D, c.dt, c.dx, c.u, c.tau
166
167     N = len(Phi)
168     Phi = np.array(Phi)
169     Phi_old = np.array(Phi)
170
171     A = D * dt / dx**2
172     B = u * dt / (8 * dx)
173
174     t = 0
175     while t <= tau:
176         for i in range(2, N - 1):
177             Phi[i] = (A * (Phi_old[i + 1] - 2 * Phi_old[i] + Phi_old[i - 1]) -
178                      B * (3 * Phi_old[i + 1] + Phi_old[i - 2] - 7 * Phi_old[i - 1] + 3 * Phi_old[i]) +
179                      Phi_old[i])
180
181             Phi[-1] = (A * (Phi_old[1] - 2 * Phi_old[-1] + Phi_old[-2]) -
182                       B * (3 * Phi_old[1] + Phi_old[-3] - 7 * Phi_old[-2] + 3 * Phi_old[-1]) +
183                       Phi_old[-1])
184             Phi[0] = Phi[-1]
185             Phi[1] = (A * (Phi_old[2] - 2 * Phi_old[1] + Phi_old[0]) -
186                      B * (3 * Phi_old[2] + Phi_old[-2] - 7 * Phi_old[0] + 3 * Phi_old[1]) +
187                      Phi_old[1])
188
189         # Increment
190         Phi_old = np.array(Phi)
191         t += dt
192
193     return np.array(Phi_old)
194
195
196 def save_figure(x, analytic, solution, title, stable):
197     plt.figure(figsize=fig_dims)
198
199     plt.plot(x, analytic, label='Analytic')
200     plt.plot(x, solution, '.', label=title.split(' ')[0])
201
202     # Calculate NRMS for this solution
203     err = solution - analytic
204     NRMS = np.sqrt(np.mean(np.square(err))) / (max(analytic) - min(analytic))
205

```



```

206 plt.ylabel('$\Phi$')
207 plt.xlabel('L (m)')
208
209 if stable:
210     stability = 'Stable, '
211 else:
212     stability = 'Unstable, '
213
214 plt.title(stability +
215           'C=' + title.split(' ')[1] +
216           ' s=' + title.split(' ')[2] +
217           ' NRMS={0:.3e}'.format(NRMS))
218 plt.legend(loc='best')
219
220 # Save plots
221 save_name = title + '.pdf'
222 try:
223     os.mkdir('figures')
224 except Exception:
225     pass
226
227 plt.savefig('figures/' + save_name, bbox_inches='tight')
228 plt.close()
229
230
231 def save_state(x, analytic, solutions, state):
232     plt.figure(figsize=fig_dims)
233
234     plt.plot(x, analytic, 'k', label='Analytic')
235     for solution in solutions:
236         plt.plot(x, solution[0], '.', label=solution[1])
237
238     plt.ylabel('$\Phi$')
239     plt.xlabel('L (m)')
240
241     title = 'C=' + state.split(' ')[0] + ' s=' + state.split(' ')[1]
242     plt.title(title)
243     plt.legend(loc='best')
244
245     # Save plots
246     save_name = title + '.pdf'
247     try:
248         os.mkdir('figures')
249     except Exception:
250         pass
251
252     plt.savefig('figures/' + save_name, bbox_inches='tight')
253     plt.close()
254
255
256 def save_state_error(x, analytic, solutions, state):
257     plt.figure(figsize=fig_dims)
258
259     for solution in solutions:
260         Error = solution[0] - analytic
261         plt.plot(x, Error, '.', label=solution[1])
262
263     plt.ylabel('Error')
264     plt.xlabel('L (m)')
265     plt.ylim([-0.05, 0.05])
266
267     title = 'C=' + state.split(' ')[0] + ' s=' + state.split(' ')[1]
268     plt.title(title)
269     plt.legend(loc='best')
270
271     # Save plots
272     save_name = 'Error ' + title + '.pdf'
273     try:
274         os.mkdir('figures')

```

```

275     except Exception:
276         pass
277
278     plt.savefig('figures/' + save_name, bbox_inches='tight')
279     plt.close()
280
281
282 def plot_order(x, t, RMS):
283     fig = plt.figure(figsize=fig_dims)
284
285     RMS, title = RMS[0], RMS[1]
286
287     # Find effective order of accuracy
288     order_accuracy_x = effective_order(x, RMS)
289     order_accuracy_t = effective_order(t, RMS)
290     # print(title, 'x order: ', order_accuracy_x, 't order: ', order_accuracy_t)
291
292     # Show effect of dx on RMS
293     fig.add_subplot(2, 1, 1)
294     plt.plot(x, RMS, '.')
295     plt.title('dx vs RMS, effective order {0:1.2f}'.format(order_accuracy_x))
296     plt.xscale('log')
297     plt.yscale('log')
298     plt.xlabel('dx')
299     plt.ylabel('NRMS')
300     fig.subplots_adjust(hspace=.35)
301
302     # Show effect of dt on RMS
303     fig.add_subplot(2, 1, 2)
304     plt.plot(t, RMS, '.')
305     plt.title('dt vs RMS, effective order {0:1.2f}'.format(order_accuracy_t))
306     plt.xscale('log')
307     plt.yscale('log')
308     plt.xlabel('dt')
309     plt.ylabel('NRMS')
310
311     # Slap the method name on
312     plt.suptitle(title)
313
314     # Save plots
315     save_name = 'Order ' + title + '.pdf'
316     try:
317         os.mkdir('figures')
318     except Exception:
319         pass
320
321     plt.savefig('figures/' + save_name, bbox_inches='tight')
322     plt.close()
323
324
325 def stability(c):
326     C, s, u = c.C, c.s, c.u
327
328     FTCS = C <= np.sqrt(2 * s * u) and s <= 0.5
329     Upwind = C + 2*s <= 1
330     Trapezoidal = True
331     QUICK = C <= min(2 - 4 * s, np.sqrt(2 * s))
332
333     # print('C = ', C, ' s = ', s)
334     # print('FTCS: ' + str(FTCS))
335     # print('Upwind: ' + str(Upwind))
336     # print('Trapezoidal: ' + str(Trapezoidal))
337     # print('QUICK: ' + str(QUICK))
338
339     return [FTCS, Upwind, Trapezoidal, QUICK]
340
341
342 def linear_fit(x, a, b):
343     '''Define our (line) fitting function'''

```

```

344     return a + b * x
345
346
347 def effective_order(x, y):
348     '''Find slope of log log plot to find our effective order of accuracy'''
349
350     logx = log10(x)
351     logy = log10(y)
352     out = curve_fit(linear_fit, logx, logy)
353
354     return out[0][1]
355
356
357 def calc_stability(C, s, solver):
358     results = []
359     for C_i, s_i in zip(C, s):
360         out = generate_solutions(C_i, s_i, find_order=True)
361         results.append(out)
362
363     # Sort and convert
364     results.sort(key=lambda x: x[0])
365     results = np.array(results)
366
367     # Pull out data
368     x = results[:, 0]
369     t = results[:, 1]
370     RMS_FTCS = results[:, 2]
371     RMS_Upwind = results[:, 3]
372     RMS_Trapezoidal = results[:, 4]
373     RMS_QUICK = results[:, 5]
374
375     # Plot effective orders
376     rms_list = [(RMS_FTCS, 'FTCS'),
377                 (RMS_Upwind, 'Upwind'),
378                 (RMS_Trapezoidal, 'Trapezoidal'),
379                 (RMS_QUICK, 'QUICK')]
380
381     for rms in rms_list:
382         if rms[1] == solver:
383             plot_order(x, t, rms)
384
385
386 def generate_solutions(C, s, find_order=False):
387     c = Config(C, s)
388
389     # Spit out some stability information
390     stable = stability(c)
391
392     # Initial Condition with boundary conditions
393     Phi_initial = np.sin(c.k * c.x)
394
395     # Analytic Solution
396     Phi_analytic = Analytic(c)
397
398     # Explicit Solution
399     Phi_ftcs = FTCS(Phi_initial, c)
400
401     # Upwind Solution
402     Phi_upwind = Upwind(Phi_initial, c)
403
404     # Trapezoidal Solution
405     Phi_trapezoidal = Trapezoidal(Phi_initial, c)
406
407     # QUICK Solution
408     Phi_quick = QUICK(Phi_initial, c)
409
410     # Save group comparison
411     solutions = [(Phi_ftcs, 'FTCS'),
412                  (Phi_upwind, 'Upwind'),

```

```

413         (Phi_trapezoidal, 'Trapezoidal'),
414         (Phi_quick, 'QUICK')]
415
416     if not find_order:
417         # Save individual comparisons
418         save_figure(c.x, Phi_analytic, Phi_ftcs,
419                     'FTCS ' + str(C) + ' ' + str(s), stable[0])
420         save_figure(c.x, Phi_analytic, Phi_upwind,
421                     'Upwind ' + str(C) + ' ' + str(s), stable[1])
422         save_figure(c.x, Phi_analytic, Phi_trapezoidal,
423                     'Trapezoidal ' + str(C) + ' ' + str(s), stable[2])
424         save_figure(c.x, Phi_analytic, Phi_quick,
425                     'QUICK ' + str(C) + ' ' + str(s), stable[3])
426
427         # and group comparisons
428         save_state(c.x, Phi_analytic, solutions, str(C) + ' ' + str(s))
429         save_state_error(c.x, Phi_analytic, solutions, str(C) + ' ' + str(s))
430
431     NRMS = []
432     for solution in solutions:
433         err = solution[0] - Phi_analytic
434         NRMS.append(np.sqrt(np.mean(np.square(err)))/(max(Phi_analytic) - min(Phi_analytic)))
435
436     return [c.dx, c.dt, NRMS[0], NRMS[1], NRMS[2], NRMS[3]]
437
438
439 def main():
440     # Cases
441     C = [0.1, 0.5, 2, 0.5, 0.5]
442     s = [0.25, 0.25, .25, 0.5, 1]
443     for C_i, s_i in zip(C, s):
444         generate_solutions(C_i, s_i)
445
446     # Stable values for each case to find effective order of methods
447     C = [0.10, 0.50, 0.40, 0.35, 0.5]
448     s = [0.25, 0.25, 0.25, 0.40, 0.5]
449     calc_stability(C, s, 'FTCS')
450
451     C = [0.1, 0.2, 0.3, 0.05, 0.1]
452     s = [0.4, 0.3, 0.2, 0.1, 0.1]
453     calc_stability(C, s, 'Upwind')
454
455     C = [0.5, 0.6, 0.7, 0.8, 0.9]
456     s = [0.25, 0.25, 0.25, 0.25, 0.25]
457     calc_stability(C, s, 'Trapezoidal')
458
459     C = [0.25, 0.4, 0.5, 0.6, 0.7]
460     s = [0.25, 0.25, 0.25, 0.25, 0.25]
461     calc_stability(C, s, 'QUICK')
462
463
464 if __name__ == "__main__":
465     main()

```

Listing 1: Code to create plots and solutions

```

1 import numpy as np
2 import matplotlib
3 matplotlib.use('TkAgg')
4
5 # Configure figures for production
6 WIDTH = 495.0 # the number latex spits out
7 FACTOR = 1.0 # the fraction of the width the figure should occupy
8 fig_width_pt = WIDTH * FACTOR
9
10 inches_per_pt = 1.0 / 72.27
11 golden_ratio = (np.sqrt(5) - 1.0) / 2.0 # because it looks good
12 fig_width_in = fig_width_pt * inches_per_pt # figure width in inches
13 fig_height_in = fig_width_in * golden_ratio # figure height in inches

```

```
14 fig_dims = [fig_width_in, fig_height_in] # fig dims as a list
```

Listing 2: Code to generate pretty plots