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 $D = 0.005$ m^2/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

3 Results Discussion

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.

Appendix A: Python Code

```python
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


class Config(object):
    def __init__(self, C, s):
        # Import parameters
        self.C = C
        self.s = s

        # Problem constants
        self.L = 1.                  # m
        self.D = 0.005               # m^2/s
        self.u = 0.2                 # m/s
        self.k = 2 * np.pi / self.L  # m^-1
        self.tau = 1 / (self.k ** 2 * self.D)

        # Set-up Mesh and Calculate time-step
        self.dx = self.C * self.D / (self.u * self.s)
        self.dt = self.C * self.dx / self.u
        self.x = np.append(np.arange(0, self.L, self.dx), self.L)


def Analytic(c):
    k, D, u, tau, x = c.k, c.D, c.u, c.tau, c.x

    N = len(x)
    Phi = np.array(x)

    for i in range(0, N):
        Phi[i] = np.exp(-k ** 2 * D * tau) * np.sin(k * (x[i] - u * tau))

    return np.array(Phi)


def FTCS(Phi, c):
    """
    FTCS (Explicit) - Forward-Time and central differencing for both the
    convective flux and the diffusive flux.
    """

    D, dt, dx, u, tau = c.D, c.dt, c.dx, c.u, c.tau

    N = len(Phi)
    Phi = np.array(Phi)
    Phi_old = np.array(Phi)

    t = 0
    while t < tau:
        for i in range(1, N - 1):
            Phi[i] = ((1 - 2 * D * dt / dx ** 2) * Phi_old[i] +
                      (D * dt / dx ** 2 + u * dt / (2 * dx)) * Phi_old[i - 1] +
                      (D * dt / dx ** 2 - u * dt / (2 * dx)) * Phi_old[i + 1])

        # Enforce our periodic boundary condition
        Phi[-1] = ((1 - 2 * D * dt / dx ** 2) * Phi_old[-1] +
                   (D * dt / dx ** 2 + u * dt / (2 * dx)) * Phi_old[-2] +
                   (D * dt / dx ** 2 - u * dt / (2 * dx)) * Phi_old[1])
        Phi[0] = Phi[-1]

        Phi_old = np.array(Phi)
        t += dt
```

```python

    return np.array(Phi_old)


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.
    '''

    D, dt, dx, u, tau = c.D, c.dt, c.dx, c.u, c.tau

    N = len(Phi)
    Phi = np.array(Phi)
    Phi_old = np.array(Phi)

    t = 0
    while t <= tau:
        Phi[0] = (D * dt / dx ** 2 * (Phi_old[1] - 2 * Phi_old[0] + Phi_old[-1]) -
                  u * dt / (2 * dx) * (3 * Phi_old[0] - 4 * Phi_old[-1] + Phi_old[-2]) +
                  Phi_old[0])

        Phi[1] = (D * dt / dx ** 2 * (Phi_old[2] - 2 * Phi_old[1] + Phi_old[0]) -
                  u * dt / (2 * dx) * (3 * Phi_old[1] - 4 * Phi_old[0] + Phi_old[-1]) +
                  Phi_old[1])

        for i in range(2, N - 1):
            Phi[i] = (D * dt / dx ** 2 * (Phi_old[i + 1] - 2 * Phi_old[i] + Phi_old[i - 1]) -
                      u * dt / (2 * dx) * (3 * Phi_old[i] - 4 * Phi_old[i - 1] + Phi_old[i - 2]) +
                      Phi_old[i])

        Phi[-1] = (D * dt / dx ** 2 * (Phi_old[0] - 2 * Phi_old[-1] + Phi_old[-2]) -
                   u * dt / (2 * dx) * (3 * Phi_old[-1] - 4 * Phi_old[-2] + Phi_old[-3]) +
                   Phi_old[-1])

        Phi_old = np.array(Phi)
        t += dt

    return np.array(Phi_old)


def Trapezoidal(Phi, c):
    D, dt, dx, u, tau = c.D, c.dt, c.dx, c.u, c.tau

    N = len(Phi)
    Phi = np.array(Phi)
    Phi_old = np.array(Phi)

    # Create Coefficient Matrix
    upper = [-(dt * D) / (2 * dx ** 2) + dt * u / (4 * dx) for _ in range(0, N)]
    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)]

    data = lower, main, upper
    diags = np.array([-1, 0, 1])
    matrix = sparse.spdiags(data, diags, N, N).todense()

    # Set values for cyclic boundary conditions
    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)

    # create blank b array
    b = np.array(Phi_old)

    t = 0
    while t <= tau:
        # Enforce our periodic boundary condition
        b[0] = ((dt * D / (2 * dx ** 2)) * (Phi_old[1] - 2 * Phi_old[0] + Phi_old[-1]) -
```

```
                (u * dt / (4 * dx)) * (Phi_old[1] - Phi_old[-1]) +
                Phi_old[0])

        for i in range(1, N - 1):
            b[i] = ((dt * D / (2 * dx ** 2)) * (Phi_old[i + 1] - 2 * Phi_old[i] + Phi_old[i - 1]) -
                    (u * dt / (4 * dx)) * (Phi_old[i + 1] - Phi_old[i - 1]) +
                    Phi_old[i])

        # Enforce our periodic boundary condition
        b[-1] = ((dt * D / (2 * dx ** 2)) * (Phi_old[0] - 2 * Phi_old[-1] + Phi_old[-2]) -
                 (u * dt / (4 * dx)) * (Phi_old[0] - Phi_old[-2]) +
                 Phi_old[-1])

        # Solve matrix
        Phi = np.linalg.solve(matrix, b)

        Phi_old = np.array(Phi)
        t += dt

    return np.array(Phi_old)


def QUICK(Phi, c):
    D, dt, dx, u, tau = c.D, c.dt, c.dx, c.u, c.tau

    N = len(Phi)
    Phi = np.array(Phi)
    Phi_old = np.array(Phi)

    t = 0
    while t <= tau:
        Phi[0] = (dt * D / dx ** 2 * (Phi_old[1] - 2 * Phi_old[0] + Phi_old[N - 1]) -
                  dt * u / (8 * dx) * (3 * Phi_old[1] + Phi_old[-2] - 7 * Phi_old[N - 1] + 3 * Phi_old[0]) +
                  Phi_old[0])
        Phi[1] = (dt * D / dx ** 2 * (Phi_old[2] - 2 * Phi_old[1] + Phi_old[0]) -
                  dt * u / (8 * dx) * (3 * Phi_old[2] + Phi_old[N - 1] - 7 * Phi_old[0] + 3 * Phi_old[1]) +
                  Phi_old[1])

        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]) -
                      dt * u / (8 * dx) * (3 * Phi_old[i + 1] + Phi_old[i - 2] - 7 * Phi_old[i - 1] + 3 * Phi_old[i])
                      Phi_old[i])

        Phi[-1] = (dt * D / dx ** 2 * (Phi_old[0] - 2 * Phi_old[-1] + Phi_old[-2]) -
                   dt * u / (8 * dx) * (3 * Phi_old[0] + Phi_old[-3] - 7 * Phi_old[-2] + 3 * Phi_old[-1]) +
                   Phi_old[-1])

        # Increment
        Phi_old = np.array(Phi)
        t += dt

    return np.array(Phi_old)


def save_figure(x, analytic, solution, title, stable):
    plt.plot(x, analytic, label='Analytic')
    plt.plot(x, solution, '.', label=title.split(' ')[0])

    # Calculate NRMS for this solution
    err = solution - analytic
    NRMS = np.sqrt(np.mean(np.square(err)))/(max(analytic) - min(analytic))

    plt.ylabel('$\Phi$')
    plt.xlabel('L (m)')

    if stable:
        stability = 'Stable, '
    else:
        stability = 'Unstable, '
```

```python

    plt.title(stability +
              'C=' + title.split(' ')[1] +
              ' s=' + title.split(' ')[2] +
              ' NRMS={0:.3e}'.format(NRMS))
    plt.legend(loc='best')

    # Save plots
    save_name = title + '.pdf'
    try:
        os.mkdir('figures')
    except Exception:
        pass

    plt.savefig('figures/' + save_name, bbox_inches='tight')
    plt.clf()


def save_state(x, analytic, solutions, state):
    plt.plot(x, analytic, 'k', label='Analytic')
    for solution in solutions:
        plt.plot(x, solution[0], '.', label=solution[1])

    plt.ylabel('$\Phi$')
    plt.xlabel('L (m)')

    title = 'C=' + state.split(' ')[0] + ' s=' + state.split(' ')[1]
    plt.title(title)
    plt.legend(loc='best')

    # Save plots
    save_name = title + '.pdf'
    try:
        os.mkdir('figures')
    except Exception:
        pass

    plt.savefig('figures/' + save_name, bbox_inches='tight')
    plt.clf()


def save_state_error(x, analytic, solutions, state):
    for solution in solutions:
        Error = solution[0] - analytic
        plt.plot(x, Error, '.', label=solution[1])

    plt.ylabel('Error')
    plt.xlabel('L (m)')
    plt.ylim([-0.05, 0.05])

    title = 'C=' + state.split(' ')[0] + ' s=' + state.split(' ')[1]
    plt.title(title)
    plt.legend(loc='best')

    # Save plots
    save_name = 'Error ' + title + '.pdf'
    try:
        os.mkdir('figures')
    except Exception:
        pass

    plt.savefig('figures/' + save_name, bbox_inches='tight')
    plt.clf()


def plot_order(x, t, RMS):
    fig = plt.figure()
    RMS, title = RMS[0], RMS[1]

```

```python
    # Find effective order of accuracy
    order_accuracy_x = effective_order(x, RMS)
    order_accuracy_t = effective_order(t, RMS)
    # print(title, 'x order: ', order_accuracy_x, 't order: ', order_accuracy_t)

    # Show effect of dx on RMS
    fig.add_subplot(2, 1, 1)
    plt.plot(x, RMS, '.')
    plt.title('dx vs RMS, effective order {0:1.2f}'.format(order_accuracy_x))
    plt.xscale('log')
    plt.yscale('log')
    plt.xlabel('dx')
    plt.ylabel('NRMS')
    fig.subplots_adjust(hspace=.35)

    # Show effect of dt on RMS
    fig.add_subplot(2, 1, 2)
    plt.plot(t, RMS, '.')
    plt.title('dt vs RMS, effective order {0:1.2f}'.format(order_accuracy_t))
    plt.xscale('log')
    plt.yscale('log')
    plt.xlabel('dt')
    plt.ylabel('NRMS')

    # Slap the method name on
    plt.suptitle(title)

    # Save plots
    save_name = 'Order ' + title + '.pdf'
    try:
        os.mkdir('figures')
    except Exception:
        pass

    plt.savefig('figures/' + save_name, bbox_inches='tight')
    plt.clf()


def stability(c):
    C, s, D, u, dx, dt = c.C, c.s, c.D, c.u, c.dx, c.dt

    FTCS = dx < (2 * D) / u and dt < dx ** 2 / (2 * D)
    FTCS = C <= np.sqrt(2 * s * u) and s <= 0.5
    Upwind = C + 2*s < 1
    Trapezoidal = True
    QUICK = C < min(2-4*s, np.sqrt(2*s))

    # print('C = ', C, ' s = ', s)
    # print('FTCS: ' + str(FTCS))
    # print('Upwind: ' + str(Upwind))
    # print('Trapezoidal: ' + str(Trapezoidal))
    # print('QUICK: ' + str(QUICK))

    return [FTCS, Upwind, Trapezoidal, QUICK]


def linear_fit(x, a, b):
    '''Define our (line) fitting function'''
    return a + b * x


def effective_order(x, y):
    '''Find slope of log log plot to find our effective order of accuracy'''

    logx = log10(x)
    logy = log10(y)
    out = curve_fit(linear_fit, logx, logy)

    return out[0][1]
```

```python


def calc_stability(C, s, solver):
    results = []
    for C_i, s_i in zip(C, s):
        out = generate_solutions(C_i, s_i, find_order=True)
        results.append(out)

    # Sort and convert
    results.sort(key=lambda x: x[0])
    results = np.array(results)

    # Pull out data
    x = results[:, 0]
    t = results[:, 1]
    RMS_FTCS = results[:, 2]
    RMS_Upwind = results[:, 3]
    RMS_Trapezoidal = results[:, 4]
    RMS_QUICK = results[:, 5]

    # Plot effective orders
    rms_list = [(RMS_FTCS, 'FTCS'),
                (RMS_Upwind, 'Upwind'),
                (RMS_Trapezoidal, 'Trapezoidal'),
                (RMS_QUICK, 'QUICK')]

    for rms in rms_list:
        if rms[1] == solver:
            plot_order(x, t, rms)


def generate_solutions(C, s, find_order=False):
    c = Config(C, s)

    # Spit out some stability information
    stable = stability(c)

    # Initial Condition with boundary conditions
    Phi_initial = np.sin(c.k * c.x)

    # Analytic Solution
    Phi_analytic = Analytic(c)

    # Explicit Solution
    Phi_ftcs = FTCS(Phi_initial, c)

    # Upwind Solution
    Phi_upwind = Upwind(Phi_initial, c)

    # Trapezoidal Solution
    Phi_trapezoidal = Trapezoidal(Phi_initial, c)

    # QUICK Solution
    Phi_quick = QUICK(Phi_initial, c)

    # Save group comparison
    solutions = [(Phi_ftcs, 'FTCS'),
                 (Phi_upwind, 'Upwind'),
                 (Phi_trapezoidal, 'Trapezoidal'),
                 (Phi_quick, 'QUICK')]

    if not find_order:
        # Save individual comparisons
        save_figure(c.x, Phi_analytic, Phi_ftcs,
                    'FTCS ' + str(C) + ' ' + str(s), stable[0])
        save_figure(c.x, Phi_analytic, Phi_upwind,
                    'Upwind ' + str(C) + ' ' + str(s), stable[1])
        save_figure(c.x, Phi_analytic, Phi_trapezoidal,
                    'Trapezoidal ' + str(C) + ' ' + str(s), stable[2])
```

```python
        save_figure(c.x, Phi_analytic, Phi_quick,
                    'QUICK ' + str(C) + ' ' + str(s), stable[3])

        # and group comparisons
        save_state(c.x, Phi_analytic, solutions, str(C) + ' ' + str(s))
        save_state_error(c.x, Phi_analytic, solutions, str(C) + ' ' + str(s))

    NRMS = []
    for solution in solutions:
        err = solution[0] - Phi_analytic
        NRMS.append(np.sqrt(np.mean(np.square(err)))/(max(Phi_analytic) - min(Phi_analytic)))

    return [c.dx, c.dt, NRMS[0], NRMS[1], NRMS[2], NRMS[3]]


def main():
    # Cases
    C = [0.1,   0.5,   2, 0.5, 0.5]
    s = [0.25, 0.25, .25, 0.5,   1]
    for C_i, s_i in zip(C, s):
        generate_solutions(C_i, s_i)

    # Stable values for each case to find effective order of methods
    C = [0.10, 0.50, 0.40, 0.35, 0.5]
    s = [0.25, 0.25, 0.25, 0.40, 0.5]
    calc_stability(C, s, 'FTCS')

    C = [0.1, 0.2, 0.3, 0.05, 0.1]
    s = [0.4, 0.3, 0.2, 0.15, 0.1]
    calc_stability(C, s, 'Upwind')

    C = [0.5, 0.6, 0.7, 0.8, 0.9]
    s = [0.25, 0.25, 0.25, 0.25, 0.25]
    calc_stability(C, s, 'Trapezoidal')

    C = [0.25, 0.4, 0.5, 0.6,  0.7]
    s = [0.25, 0.25, 0.25, 0.25, 0.25]
    calc_stability(C, s, 'QUICK')


if __name__ == "__main__":
    main()
```

Listing 1: Code to create plots and solutions

```python
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