Case Study # 1: 1D Transient Heat Diffusion

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1 Problem Description

The problem of 1D unsteady heat diffusion in a slab of unit length with a zero initial temperature and both ends maintained at a unit temperature can be described by:

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} \text{ subject to } \begin{cases} T(x, 0^-) = 0 & \text{for } 0 \le x \le 1 \\ T(0, t) = T(1, t) = 1 & \text{for } t > 0 \end{cases}$$
(1)

and has the well known analytical solution:

$$T^*(x,t) = 1 - \sum_{k=1}^{\infty} \frac{4}{(2k-1)\pi} \sin[(2k-1)\pi x] \star \exp[-(2k-1)^2 \pi^2 t].$$
 (2)

In addition to the analytical solution, several numerical methods can be employed to solve the diffusion equation. Two of these methods are derived in the following section.

2 Solution Algorithms

The Taylor-series (TS) method can be used on this equation to derive a finite difference approximation to the PDE. Applying the definition of the derivative,

$$f'(x) \approx \frac{f(x+\varepsilon) - f(x)}{\varepsilon}$$
 (3)

to Eqn. (1) yields

$$\frac{\partial T}{\partial t} = \frac{T(x, t + \Delta t) - T(x, t)}{\Delta t}$$

$$= \frac{T_i^{k+1} - T_i^k}{\Delta t}.$$
(4)

From the definition of the Taylor series,

$$f(x+\varepsilon) = f(x) + \varepsilon f'(x) + \frac{\varepsilon^2}{2} f''(x) + \dots$$
 (5)

which, when applied to T_i^{k+1} and T_i^k gives

$$T_{i+1} = T_i + \Delta x \frac{\partial T_i}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 T_i}{\partial x^2} + \mathcal{O}(\Delta x^3)$$
 (6)

and

$$T_{i-1} = T_i - \Delta x \frac{\partial T_i}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 T_i}{\partial x^2} - O(\Delta x^3). \tag{7}$$

Adding Eqn. (6) and Eqn. (7) yields

$$T_{i+1} + T_{i-1} = 2T_i + \Delta x^2 \frac{\partial^2 T_i}{\partial x^2} + \mathcal{O}(\Delta x^4)$$
 (8)

which can be rearranged as the approximation for the second order term from Eqn. (1),

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1} + 2T_i + T_{i-1}}{\Delta x^2} + O(\Delta x^4),\tag{9}$$

and can also be combined with the above equations to form

$$\frac{T_i^{k+1} - T_i^k}{\Delta t} \approx \frac{T_{i+1}^k - 2T_i^k + T_{i-1}^k}{\Delta x^2}.$$
 (10)

This result can be arranged to form both Forward-Time, Centered-Space (FTCS) explicit and implicit schemes.

2.1 Explicit

Eqn. (10) can be rearranged to form the explicit scheme, which is

$$T_i^{k+1} = sT_{i+1}^k + (1-2s)T_i^k + sT_i^k \tag{11}$$

where

$$s = \frac{\alpha \Delta t}{\Delta x^2} \tag{12}$$

and α is the thermal diffusivity of the material.

This scheme can be implemented to solve the problem computationally. In pseudocode, looks like

$$\begin{aligned} \textbf{while } t &\leq t_{end} \ \textbf{do} \\ & \text{$i \leftarrow 1$} \\ & \textbf{for } i \text{ in } N-1 \ \textbf{do} \\ & T_{k+1}[i] = sT_k[i+1] + (1-2s)T_k[i] + sT_k[i-1] \\ & \text{$i \leftarrow i+1$} \\ & \textbf{end for} \\ & T_k = T_{k+1} \\ & \text{$t \leftarrow t+dt$} \\ & \textbf{end while} \end{aligned}$$

where N is the number of elements in your mesh. Each element in the interior is looped over (the boundary conditions remain constant), and the time marches forward until the designated end time has been reached.

2.2 Implicit

Eqn. (10) can also be rearranged to form the implicit scheme, which is

$$T_i^k = -sT_{i+1}^{k+1} + (1+2s)T_i^{k+1} - sT_{i-1}^k$$
 (13)

where again,

$$s = \frac{\alpha \Delta t}{\Delta x^2} \tag{14}$$

and α is the thermal diffusivity of the material.

This scheme can also be implemented to solve the problem computationally. In pseudocode, this is

```
\begin{array}{l} \textbf{if } i \geq maxval \textbf{ then} \\ i \leftarrow 0 \\ \textbf{else} \\ \textbf{if } i+k \leq maxval \textbf{ then} \\ i \leftarrow i+k \\ \textbf{end if} \\ \textbf{end if} \end{array}
```

3 Results

A Python script was used to obtain results for a 21 point mesh (N=21), and the Root Mean Square error,

RMS =
$$\frac{1}{N^2} \sqrt{\sum_{i=1}^{N} [T_i^n - T^*(x_i, t_n)]^2}$$
 (15)

was obtained for $s(=\Delta t/\Delta x^2) = 1/6$, 0.25, 0.5, and 0.75, at t = 0.03, 0.06, and 0.09 using both the explicit and the implicit methods.

t	Explicit RMS	Implicit RMS
0.03	4.41E-4	3.46E-5
0.06	5.66E-4	3.33E-6
0.09	6.26E-4	9.44E-6

Table 1. RMS results from the numerical simulations compared to the analytic solution for s = 1/6

t	Explicit RMS	Implicit RMS
0.03	6.59E-4	2.24E-5
0.06	9.05E-4	6.06E-6
0.09	9.61E-4	9.35E-6

Table 2. RMS results from the numerical simulations compared to the analytic solution for s=0.25

t	Explicit RMS	Implicit RMS
0.03	1.74E-3	3.77E-5
0.06	2.24E-3	1.53E-5
0.09	2.21E-3	1.95E-5

Table 3. RMS results from the numerical simulations compared to the analytic solution for s=0.5

t	Explicit RMS	Implicit RMS
0.03	3.87E-3	5.38E-5
0.06	4.21E-3	2.46E-5
0.09	3.51E-3	2.96E-5

Table 4. RMS results from the numerical simulations compared to the analytic solution for s = 0.75

The RMS between the implicit and analytic solutions and the explicit and analytic solutions are shown in Table 3. The RMS tended to grow as a function of s, and shrink as a function of t. Additionally, the RMS for the explicit solution tended to be two orders of magnitude larger than the RMS for the implicit solution.

4 Discussions

Shankle chicken tail, fatback short ribs meatball pancetta ball tip sirloin short loin. Pork tongue pork belly pork loin beef ribs. Shank turkey pork belly pork loin ham hock ball tip leberkas meatloaf chuck ground round filet mignon kielbasa sirloin turducken tri-tip. Pancetta brisket sirloin beef ribs spare ribs, swine bacon ham hock. Ham kielbasa corned beef turkey turducken. Kevin biltong pork,

tenderloin chuck pig ball tip filet mignon.

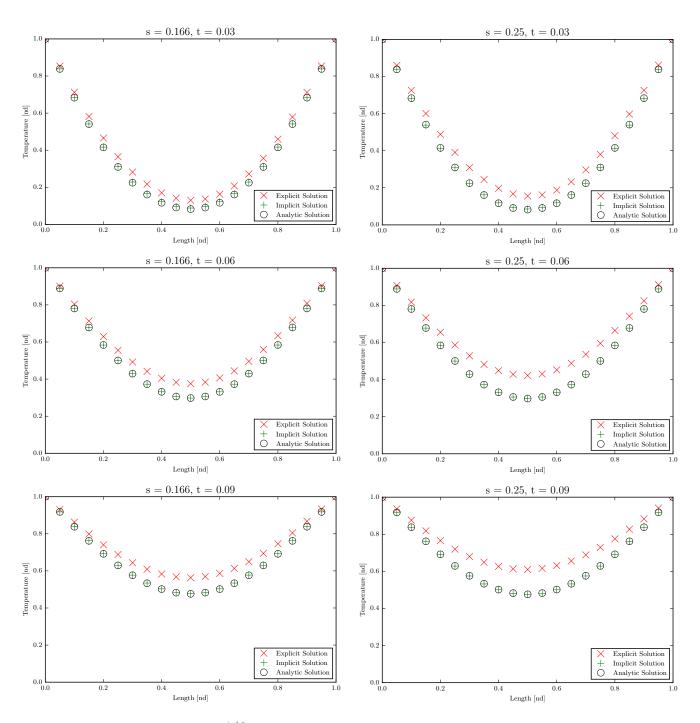


Fig. 1. Results for s = 1/6

Fig. 2. Results for s = 0.25

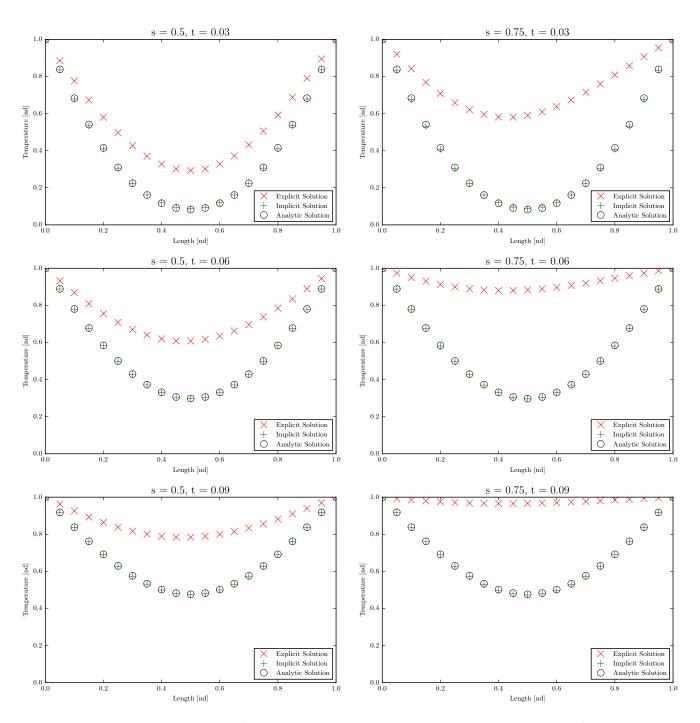


Fig. 3. Results for s=0.5

Fig. 4. Results for s = 0.75

```
1 import numpy as np
 2 import matplotlib.pyplot as plt
 3 import os
 5 # Configure figures for production
 6 WIDTH = 495.0 # the number latex spits out
 7 FACTOR = 1.0 # the fraction of the width you'd like the figure to occupy
 8 fig_width_pt = WIDTH * FACTOR
10 inches_per_pt = 1.0 / 72.27
11 golden_ratio = (np.sqrt(5) - 1.0) / 2.0 # because it looks good
12
13 fig_width_in = fig_width_pt * inches_per_pt # figure width in inches
14 fig_height_in = fig_width_in * golden_ratio # figure height in inches
                = [fig_width_in, fig_height_in] # fig dims as a list
15 fig_dims
17
18 def Solver(s, t_end, show_plot=False):
19
      # Problem Parameters
                           # Domain lenghth [n.d.]
# Initial temperature [n.d.]
        L = 1. # Domain lenghth
21
        T0 = 0.
                          # Boundary temperature [n.d.]
        T1 = 1.
22
23
        N = 21
24
25
        # Set-up Mesh
26
        x = np.linspace(0, L, N)
27
        dx = x[1] - x[0]
28
29
        # Calculate time-step
        dt = s * dx ** 2.0
30
31
32
        # Initial Condition with boundary conditions
33
        T_initial = [T0] * N
        T_initial[0] = T1
34
        T_{initial[N-1]} = T1
35
36
37
        # Explicit Numerical Solution
        T_explicit = Explicit(np.array(T_initial).copy(), t_end, dt, s)
39
        # Implicit Numerical Solution
40
        T_implicit = Implicit(np.array(T_initial).copy(), t_end, dt, s)
41
42
43
        # Analytical Solution
44
        T_analytic = np.array(T_initial).copy()
        for i in range(0, N):
45
            T_analytic[i] = Analytic(x[i], t_end)
46
47
        # Find the RMS
48
        RMS = RootMeanSquare(T implicit, T analytic)
49
50
        ExplicitRMS = RootMeanSquare(T_explicit, T_analytic)
51
52
        # Format our plots
53
        plt.figure(figsize=fig_dims)
54
        plt.axis([0, L, T0, T1])
55
        plt.xlabel('Length [nd]')
        plt.ylabel('Temperature [nd]')
        plt.title('s = ' + str(s)[:5] + ', t = ' + str(t_end)[:4])
57
58
59
        # ...and finally plot
        plt.plot(x, T_explicit, 'xr', markersize=9, label='Explicit Solution')
plt.plot(x, T_implicit, '+g', markersize=9, label='Implicit Solution')
plt.plot(x, T_analytic, 'ob', markersize=9, mfc='none', label='Analytic Solution')
60
61
62
63
        plt.legend(loc='lower right')
64
65
        save_name = 'proj_1_s_' + str(s)[:5] + '_t_' + str(t_end) + '.pdf'
66
```

```
67
 68
            os.mkdir('figures')
         except Exception:
 69
 70
            pass
 71
         plt.savefig('figures/' + save_name, bbox_inches='tight')
 72
 73
         if show_plot:
 74
             plt.show()
 75
         plt.clf()
 76
 77
         return RMS, ExplicitRMS
 78
 79
 80 def Explicit(Told, t_end, dt, s):
 81
 82
         This function computes the Forward-Time, Centered-Space (FTCS) explicit
 83
         scheme for the 1D unsteady heat diffusion problem.
 84
 85
         N = len(Told)
 86
         time = 0.
         Tnew = Told
 87
 88
         while time <= t end:</pre>
 89
             for i in range(1, N - 1):
    Tnew[i] = s * Told[i + 1] + (1 - 2.0 * s) * Told[i] + s * Told[i - 1]
 90
 91
 92
 93
             Told = Tnew
 94
             time += dt
 95
 96
         return Told
 97
98
99 def Implicit(Told, t_end, dt, s):
100
         This function computes the Forward-Time, Centered-Space (FTCS) implicit
101
102
         scheme for the 1D unsteady heat diffusion problem.
103
         N = len(Told)
104
105
         time = 0.
106
         # Build our 'A' matrix
107
        a = [-s] * N
a[0], a[-1] = 0, 0
108
109
         b = [1 + 2 * s] * N
110
111
         b[0], b[-1] = 1, 1
                                  # hold boundary
112
113
         while time <= t end:</pre>
114
             Tnew = TDMAsolver(a, b, c, Told)
115
116
             Told = Tnew
time += dt
117
118
119
120
         return Told
121
122
123 def RootMeanSquare(a, b):
124
125
         This function will return the RMS between two lists (but does no checking
126
         to confirm that the lists are the same length).
127
         N = len(a)
128
129
130
         RMS = 0.
131
         for i in range(0, N):
132
            RMS += (a[i] - b[i]) ** 2.
133
```

```
134
        RMS = RMS ** (1. / 2.)
135
        RMS /= N**2.
136
137
        return RMS
138
139
140 def TDMAsolver(a, b, c, d):
141
142
         Tridiagonal Matrix Algorithm (a.k.a Thomas algorithm).
143
144
        N = len(a)
        Tnew = d
145
146
        # Initialize arrays
147
148
        gamma = np.zeros(N)
149
        xi = np.zeros(N)
150
151
        # Step 1
152
        gamma[0] = c[0] / b[0]
153
        xi[0] = d[0] / b[0]
154
155
        for i in range(1, N):
             gamma[i] = c[i] / (b[i] - a[i] * gamma[i - 1])
156
             xi[i] = (d[i] - a[i] * xi[i - 1]) / (b[i] - a[i] * gamma[i - 1])
157
158
159
         # Step 2
160
        Tnew[N - 1] = xi[N - 1]
161
         for i in range(N - 2, -1, -1):
162
            Tnew[i] = xi[i] - gamma[i] * Tnew[i + 1]
163
164
165
        return Tnew
166
167
168 def Analytic(x, t):
169
170
         The analytic answer is 1 - Sum(terms). Though there are an infinite
171
         number of terms, only the first few matter when we compute the answer.
172
173
        result = 1
        large_number = 1E6
174
175
176
        for k in range(1, int(large_number) + 1):
            term = (4. / ((2. * k - 1.) * np.pi)) * np.sin((2. * k - 1.) * np.pi * x) *
177
178
                     np.exp(-(2. * k - 1.) ** 2. * np.pi ** 2. * t))
179
180
181
             # If subtracting the term from the result doesn't change the result
             # then we've hit the computational limit, else we continue.
182
             # print '{0} {1}, {2:.15f}'.format(k, term, result)
183
             if result - term == result:
184
185
                return result
             else:
186
187
                 result -= term
188
189
190 def main():
191
        Main function to call solver over assigned values and create some plots to
192
193
        look at the trends in RMS compared to s and t.
194
        \# Loop over requested values for s and t
195
196
        s = [1. / 6., .25, .5, .75]
        t = [0.03, 0.06, 0.09]
197
198
199
        RMS = []
        with open('results.dat', 'w+') as f:
200
```

```
for i, s_ in enumerate(s):
    sRMS = [0] * len(t)
201
202
                   for j, t_ in enumerate(t):
203
204
                        sRMS[j], ExplicitRMS = Solver(s_, t_, False)
                        205
206
                        # print i, j, sRMS[j]
207
                   RMS.append(sRMS)
208
209
          # Convert to np array to make this easier...
210
          RMS = np.array(RMS)
211
          # Check for trends in RMS vs t
212
213
          plt.figure(figsize=fig_dims)
         plt.ligure(ligs1ze=lig_dims)
plt.plot(t, RMS[0], '.r', label='s = 1/6')
plt.plot(t, RMS[1], '.g', label='s = .25')
plt.plot(t, RMS[2], '.b', label='s = .50')
plt.plot(t, RMS[3], '.k', label='s = .75')
214
215
216
217
218
          plt.xlabel('t')
          plt.ylabel('RMS')
219
220
          plt.title('RMS vs t')
          plt.legend(loc='best')
221
222
          save_name = 'proj_1_rms_vs_t.pdf'
223
          plt.savefig('figures/' + save_name, bbox_inches='tight')
224
225
          plt.clf()
226
227
          # Check for trends in RMS vs s
228
          plt.figure(figsize=fig_dims)
         plt.plot(s, RMS[:, 0], '.r', label='t = 0.03')
plt.plot(s, RMS[:, 1], '.g', label='t = 0.06')
plt.plot(s, RMS[:, 2], '.b', label='t = 0.09')
229
230
231
232
          plt.xlabel('s')
          plt.ylabel('RMS')
233
234
          plt.title('RMS vs s')
235
          plt.legend(loc='best')
236
237
          save_name = 'proj_1_rms_vs_s.pdf'
238
          plt.savefig('figures/' + save_name, bbox_inches='tight')
239
          plt.clf()
240
241 if __name__ == "__main__":
242
          main()
```