Computational Methods & C++ Assignment

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${f Abstract}$			
A one-space dimensional problem is considered, to examine the appli- cation of numerical schemes for the solution of partial differential equa- tions.			

1 Introduction

2 Methods

Several methods are used:

- Dufort-Frankel
- Richardson
- Laasonen simple implicit
- Crank-Nicholson

For all of the used schemes, the initialization of the result matrix is run the same way. First the study grid must be chosen. The initials conditions are:

- T_{int} of 100° F
- T_{sur} of 300°F
- $D = 0.1 ft^2/hr$

First it was assumed that $\Delta x = 0.05$ and $\Delta t = 0.01$, so that the result matrix could be initialized. We set:

$$n_{space} = \frac{L}{\Delta x} + 1 \tag{1}$$

$$n_{time} = \frac{T}{\Delta t} \tag{2}$$

 n_{space} is the number of iterations over the grid, according to the coordinate x. n_{time} is the number of iterations over the grid, according to the time t.

This is how the matrix is initialized, according to initial conditions. For most of the used schemes, we need two previous time steps to calculate the current step. An order one scheme is used to find the second line of the matrix:

$$T_{i,1} = \frac{\alpha}{2} (T_{i+1,0} + T_{i-1,0}) + (1 - \alpha) T_{i,0}$$
(3)

with

$$\alpha = 2 \frac{D\delta t}{\delta x^2}$$

So we have:

$$\begin{aligned} i &= 0 & i &= 1 & \cdots & n_{space} - 1 & n_{space} \\ \begin{pmatrix} T_{ext} & T_{int} & \cdots & T_{int} & T_{ext} \\ T_{ext} & T_{i,1} & \cdots & T_{i,1} & T_{ext} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ T_{ext} & 0 & \cdots & 0 & T_{ext} \end{pmatrix} \begin{matrix} j &= 0 \\ j &= 1 \\ \vdots \\ n_{time} \end{matrix}$$

With this trick our matrix is ready to be used and filled up with every scheme.

2.1 Explicit schemes

For both of the explicit schemes used (Dufort-Frankel and Richardson schemes), the solving is run the same way : with a double for-loop, the matrix is filled up. The only thing that change is the way we advance in time and space.

2.1.1 Dufort-Frankel

Explicitly, for Dufort-Frankel method, we have:

$$T_j^{n+1} = \left(\frac{1-\alpha}{1+\alpha}\right)T_j^{n-1} + \left(\frac{\alpha}{1+\alpha}\right)(T_{j+1}^n + T_{j-1}^n) \tag{4}$$

with

$$\alpha = 2\frac{D\delta t}{\delta x^2}$$

2.1.2 Richardson

Explicitly, for Richardson method, we have:

$$T_j^{n+1} = T_j^{n-1} + \alpha (T_{j-1}^n - 2T_j^n + T_{j+1}^n)$$
 (5)

with

$$\alpha = 2 \frac{D\delta t}{\delta x^2}$$

2.2 Implicit schemes

For both implicit schemes, the vector solution is given by a matrix equation. A LU factorization is used once, before a for-loop, to resolve the system for each space step.

2.2.1 Laasonen

We have :

$$\frac{T_j^{n+1} - T_j^n}{\Delta t} = D \frac{T_{j+1}^{n+1} - 2T_j^{n+1} + T_{j-1}^{n+1}}{\Delta x^2}$$
 (6)

Written in a matrical way, the solution at space step n+1 is given by:

$$\begin{bmatrix} 1 + 2C & -C & 0 & \cdots & 0 \\ -C & 1 + 2C & -C & \ddots & \vdots \\ 0 & -C & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 1 + 2C & -C \\ 0 & \cdots & 0 & -C & 1 + 2C \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_i \\ \vdots \\ T_{ntime} \end{bmatrix}_{n+1} = \begin{bmatrix} T_1 + CT_0 \\ T_2 \\ \vdots \\ T_i \\ \vdots \\ T_{ntime} + CT_f \end{bmatrix}_n$$
(7)

with

$$C = \frac{D\Delta t}{\Delta x^2}$$

The first vector at space n is our boundaries conditions vector, so it is known. In this scheme we must be aware that the right-term vector is actually bigger than the other, of 2 values, which corresponds to the exterior temperatures, which stays the same all the time.

We apply the LU solve algorithm for each space step, at the reduced vector, and add the n+1 vector to our result matrix. The new right term vector is the one found with the LU solve algorithm.

2.2.2 Crank-Nicholson

We have:

$$\frac{T_j^{n+1} - T_j^n}{\Delta t} = D \frac{1}{2} \left(\frac{T_{j+1}^{n+1} - 2T_j^{n+1} + T_{j-1}^{n+1}}{\Delta x^2} + \frac{T_{j+1}^n - 2T_j^n + T_{j-1}^n}{\Delta x^2} \right)$$
(8)

Written in a matrical way, the solution at space step n+1 is given by :

$$\begin{bmatrix} 1+C & -C/2 & 0 & \cdots & 0 \\ -C/2 & 1+C & -C/2 & \ddots & \vdots \\ 0 & -C/2 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 1+C & -C/2 \\ 0 & \cdots & 0 & -C/2 & 1+C \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_i \\ \vdots \\ T_{ntime} \end{bmatrix}$$
(9)

$$= \begin{bmatrix} 1 - C & C/2 & 0 & \cdots & 0 \\ C/2 & 1 - C & C/2 & \ddots & \vdots \\ 0 & C/2 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 1 - C & C/2 \\ 0 & \cdots & 0 & C/2 & 1 - C \end{bmatrix} \begin{bmatrix} T_1 + CT_0 \\ T_2 \\ \vdots \\ T_i \\ \vdots \\ T_{ntime} + CT_f \end{bmatrix}_{n}$$

with

$$C = \frac{D\Delta t}{\Delta x^2}$$

The method is the same as Laasonen scheme, except that the left term vector found with the LU solve algorithm is multiplied by the right term matrix before the next space step.

2.3 Object Oriented Design

The object oriented classes for the C++ code are designed the following way :

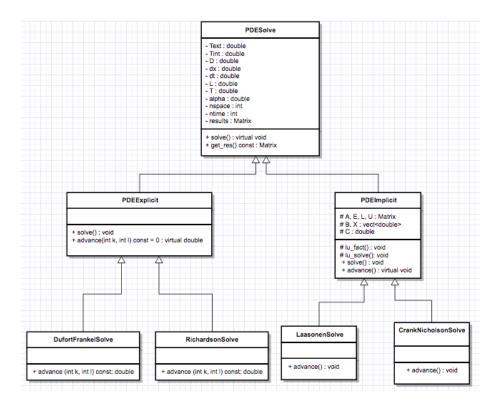


Figure 1: UML Diagram of the C++ object oriented code

There is a main base class called PDESolve, which initializes all the variables, and two functions :

- get_res(): returns the results Matrix
- solve(): virtual function which will be overwritten in subclasses

There is two subclasses of PDESolve: PDEExplicit and PDEImplicit. Each one has a solve() function, and a virtual advance function, which corresponds at the way the space and time steps are incremented. The PDEImplicit class also initializes all the matrixes and functions needed for the LU factorization and solve. Each subsubclass, which corresponds to each method, has its own particular advance method.

- 3 Results
- 3.1 Schemes study
- 3.2 Laasonen study: effect of the step time