

ID: 70040441

Computational Physics\_PHYS624 HW6: Pratial Differential Equations

\_\_\_\_\_

## Solving the Heat Diffusion Equation with the Explicit Method

#### 1. Introduction

The objective is to solve the heat diffusion differential eqaution using the explicit method

Use steps sizes (a) h = 0.1 and k = 0.0005 and (b) h = 0.1 and k = 0.01 to approximate the solution to the heat equation

$$\frac{\partial u}{\partial t}(x,t) - \frac{\partial^2 u}{\partial x^2}(x,t) = 0, \quad 0 < x < 1, \quad 0 \le t,$$

with boundary conditions

$$u(0,t) = u(1,t) = 0, \quad 0 < t,$$

and initial conditions

$$u(x,0) = \sin(\pi x), \quad 0 \le x \le 1.$$

Compare the results at t = 0.5 to the exact solution

$$u(x,t) = e^{-\pi^2 t} \sin(\pi x).$$

The Equation used for the Explicit Scheme for PDE's:

$$u_{i,j+1} = \alpha u_{i-j} + (1 - 2\alpha)u_{i,j} + \alpha u_{i+1,j}$$

#### **Script structure**

- 1. Defining the analytical function
- 2. Entering the requied data as user input for h, k, T, L.

h: the spatial step. = 0.1

k: the time step =  $\{0.0005, 0.01\}$ 

T: the total simulation time.= $\{0.5\}$ 

L: the second boundary condition. = 1

- 3. Calculating alpha = k / (h \* h)
- 4. Checking the stability condition if alpha  $\geq$ = 0.5, however the cod still runs.

A message will appear in the terminal showing that the stability is not achieved.

- 5. Creating two loops for time and position.
- 6. Saving data to (.dat) files, \_\_\_\_\_ online resources are dealing pretty much with dat files, therfore I tried that out.





ID: 70040441

Computational Physics\_PHYS624 HW6: Pratial Differential Equations

```
C++ Script
#include <iostream>
#include <cmath>
#include <iomanip>
#include <vector>
#include <fstream> // Include for file operations
using namespace std;
double h, k, T, L;
// Exact solution function
double exact solution(double x, double t) {
    if (x == 0.0 || x == L) {
        return 0.0:
    return exp(-M PI * M PI * t) * sin(M PI * x);
}
int main() {
    // Get user inputs
    cout << "Enter the spatial step size (h): ";</pre>
    cin >> h;
    cout << "Enter the time step size (k): ";</pre>
    cin >> k;
    cout << "Enter the total simulation time (T): ";</pre>
    cin >> T:
    cout << "Enter the length of the rod (L): ";</pre>
    cin >> L:
    double alpha = k / (h * h);
    // Warn about stability condition but do not terminate
    if (alpha >= 0.5) {
        cerr << "Warning: Stability condition violated (alpha >= 0.5).
Results may be inaccurate.\n";
    }
    int nx = static_cast<int>(L / h) + 1;
    int nk = static cast<int>(T / k) + 1;
    // Grid and time step indices
    int i, j;
    // Define the grid
    vector<vector<double> > u(nk, vector<double>(nx, 0.0));
pg. 2
```





ID: 70040441

Computational Physics\_PHYS624 HW6: Pratial Differential Equations

```
// Set initial and boundary conditions
    for (i = 0; i < nx; ++i) {
        double x = i * h;
        u[0][i] = sin(M PI * x / L); // Initial condition
    }
    for (j = 1; j < nk; ++j) {
        u[i][0] = 0.0;
                                 // Boundary at x=0
        u[j][0] = 0.0; // Boundary at x=0 
 u[j][nx - 1] = 0.0; // Boundary at x=L
    }
    // Time integration loop (explicit scheme)
    for (j = 0; j < nk - 1; ++j) {
        for (i = 1; i < nx - 1; ++i) {
            u[j + 1][i] = alpha * u[j][i - 1] + (1 - 2 * alpha) * u[j][i]
+ alpha * u[j][i + 1];
    }
    // Open a file to save the data
    ofstream outfile("Heat Diffusion distribution.dat");
    if (!outfile.is_open()) {
        cerr << "Error: Could not open file for writing!" << endl;
        return 1;
    }
    // Write data to file in a format suitable for plotting
    outfile << "x t u_exact u_numerical\n"; // Header</pre>
    for (j = 0; j < nk; ++j) {
        double t = j * k; // Current time
        for (i = 0; i < nx; ++i) {
            double x = i * h;
            double exact = exact_solution(x, t);
            outfile << x << " " << t << " " << exact << " " << u[j][i] <<
"\n";
        outfile << "\n"; // Separate time steps with a blank line
    }
    outfile.close();
    cout << "Data saved to temperature_distribution.dat" << endl;</pre>
    // Output results for a few selected time steps (optional)
    cout << "Numerical and Exact Solutions for selected time steps:\n";</pre>
```





ID: 70040441

Computational Physics PHYS624 **HW6: Pratial Differential Equations** 

```
cout << "----\n":
  for (j = 0; j < nk; j += nk / 10) { // Output 10 evenly spaced time}
steps
      double t = j * k; // Current time
      cout << "Time = " << t << "\n";
                   Numerical Exact Error\n";
      cout << "x
      cout << "----\n":
      for (i = 0; i < nx; ++i) {
         double x = i * h;
         double exact = exact solution(x, t);
         double error = abs(u[j][i] - exact);
         cout << setw(10) << x
            << setw(15) << u[j][i]
            << setw(15) << exact
            << setw(15) << error << "\n";
      cout << "----\n":
   }
   return 0;
}
```

\*\*\*The script calcuates the numerical and the exact vlaue at each timestep and corresponding position.

#### Sample of script results

At h= 0.1 and k=0.0005

Stability condition is achieved, where alpha =0.05

```
x t u exact. u numerical
0 0.5 0
                  0
0.1 0.5 0.00222241 0.00228652
0.2 0.5 0.00422728 0.00434922
0.3 0.5 0.00581836 0.00598619
0.4 0.5 0.00683989 0.00703719
0.5 0.5 0.00719188 0.00739934
0.6 0.5 0.00683989 0.00703719
0.7\ 0.5\ 0.00581836\ 0.00598619
0.8 0.5 0.00422728 0.00434922
0.9\ 0.5\ 0.00222241\ 0.00228652
1 0.5 0
```



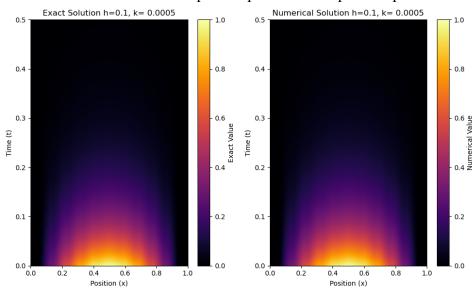
ID: 70040441

Computational Physics\_PHYS624 HW6: Pratial Differential Equations

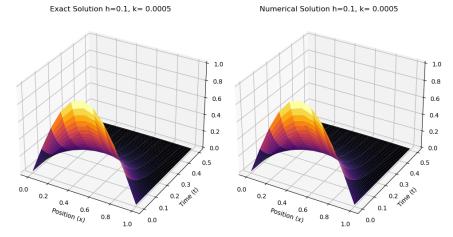
\_\_\_\_\_\_

#### **Plotting the results**

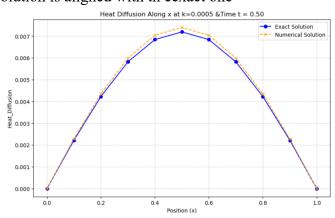
Plot1: Presents the Heat diffusion map over spatial and temporal steps



Plot2: Presents a surface plot of the same solution presented above.



Plot3: Presents the heat distribution at time step=0.5 along the x-position with as step k=0.0005. The stability condition is clear here as the numerical solution is aligned with the exact one







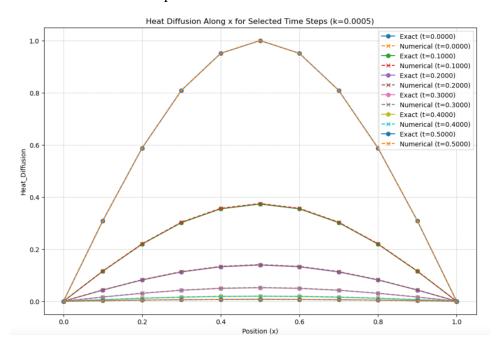
ID: 70040441

Computational Physics\_PHYS624 HW6: Pratial Differential Equations

------

# Plot4: presents a comparison of the numerical and the exact solution at different time steps.

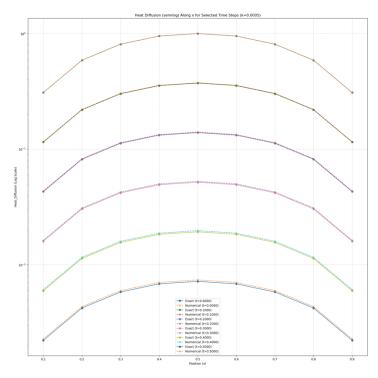
Once again the stability is clear at all those time steps.



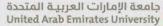
Plot5: Presents an overplot of the numerical and the exact solution in a semilog format for the heat diffusion.

This plots aims to clarify the color map(plot1) and the surface plot(plot2) mentioned above.

One cann easily understand the at the boundaries the function yields zero which is not included in the plot as log(0) is undefined, therfore I masked the results in position range((x\_values >= 0.1) & (x\_values <= 0.9))









ID: 70040441

Computational Physics PHYS624 **HW6: Pratial Differential Equations** 

#### At h = 0.1 and k = 0.01

### Stability condition is not achieved, where alpha =1

t u exact u numerical

0.5

0

0.1 0.5 0.00222241 657271

0.2 0.5 0.00422728 -1.24783e+06

0.3 0.5 0.00581836 1.71241e+06

0.4 0.5 0.00683989 -2.00552e+06

0.5 0.5 0.00719188 2.09995e+06

0.6 0.5 0.00683989 -1.98881e+06

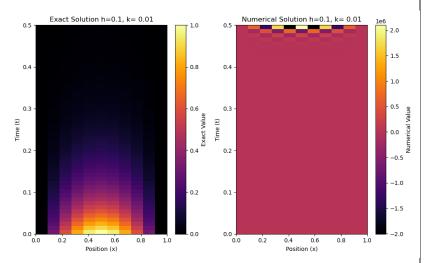
0.7 0.5 0.00581836 1.68537e+06

0.8 0.5 0.00422728 -1.22079e+06

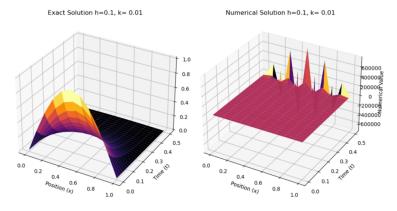
0.9 0.5 0.00222241 640558 0.50

0

Plot6: Presents the Heat diffusion map over spatial and temporal steps



Plot7: Presents a surface plot of the same solution presented above.



#### Plot8: Presents the heat distribution at time step=0.5 along the x-position with as step k=0.01

It is very clear that the solution is unstable here as the value of alpha = 1, therefore we cannot consider larger steps in the explicit scheme of solving PDE's.

