Programming Assignment 2 Report

Software Development for Scientific Computing

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PART-1

This report presents the implementation and results for Programming Assignment 2 (PA2).

```
./pa5 fine
Banded
Lower Bandwidth: 9
Upper Bandwidth: 9
The matrix is
    108333     -37500          0          0          0          0          0          0          0   -16666.7...
    -37500     108333     -37500          0          0          0          0          0          0          0
         0     -37500     108333     -37500          0          0          0          0          0          0
         0          0     -37500     108333     -37500          0          0          0          0          0
         0          0          0     -37500     108333     -37500          0          0          0          0
         0          0          0          0     -37500     108333     -37500          0          0          0
         0          0          0          0          0     -37500     108333     -37500          0          0
         0          0          0          0          0          0     -37500     108333     -37500          0
         0          0          0          0          0          0          0     -37500     108333          0
  -16666.7          0          0          0          0          0          0          0          0     108333
  ........
  ........
  so on.....
```

PART-2

The primary objective was to solve the 1D heat diffusion equation using a finite-difference approach. This involved designing three main classes:

- **RDomain**: For defining the computational domain and generating grids.
- **GridFn**: For modeling the grid function and performing updates based on the 1D heat diffusion equation.
- **Solution**: For integrating the domain and grid function, performing simulations, and analyzing convergence.

Implementation Details

Problem Setup

The heat diffusion equation was solved for a 1D rod of length $l = 1.2$ with:

- Spatial step size, $\delta x = 0.4$,
- Time step, $\delta t = 0.1$,
- Thermal diffusivity, $\alpha = 1.0$,
- Boundary conditions: $T(0) = T(l) = 0$.

The initial temperature distribution was given by $f(x) = x\sqrt{(l-x)^3}$.

Algorithm

The numerical solution used an explicit finite-difference method:

$$u(x, t + \delta t) = u(x, t) + \frac{\alpha \delta t}{\delta x^2} \left(u(x - \delta x, t) - 2u(x, t) + u(x + \delta x, t) \right).$$

The solution iterated until convergence (max error $< 10^{-6}$) or until a maximum number of steps (1000) was reached.

Simulation Workflow

The following steps were implemented:

1. Define the computational domain using **RDomain**.
2. Initialize the grid function with **GridFn**.
3. Perform iterative updates using **Solution**.
4. Monitor the maximum error for convergence.

Results

The simulation results for the given parameters are as follows:

```
./simulation 1.2 0.1 0.4
Number of grid points: 4
step 0 max error= 0.23128, Grid[0]=0, Grid[1]=0.0549369, Grid[2]=0.128289, Grid[3]=0
step 1 max error= 0.126026, Grid[0]=0, Grid[1]=0.0664464, Grid[2]=0.00226333, Grid[3]=0
step 2 max error= 0.0816434, Grid[0]=0, Grid[1]=-0.015197, Grid[2]=0.0409632, Grid[3]=0
step 3 max error= 0.0607021, Grid[0]=0, Grid[1]=0.0294012, Grid[2]=-0.0197389, Grid[3]=0
step 4 max error= 0.0490884, Grid[0]=0, Grid[1]=-0.0196871, Grid[2]=0.0233105, Grid[3]=0
step 5 max error= 0.0414426, Grid[0]=0, Grid[1]=0.0194908, Grid[2]=-0.0181321, Grid[3]=0
step 6 max error= 0.0356961, Grid[0]=0, Grid[1]=-0.0162053, Grid[2]=0.0167148, Grid[3]=0
step 7 max error= 0.0310218, Grid[0]=0, Grid[1]=0.0144981, Grid[2]=-0.014307, Grid[3]=0
step 8 max error= 0.0270645, Grid[0]=0, Grid[1]=-0.0125664, Grid[2]=0.012638, Grid[3]=0
step 9 max error= 0.0236515, Grid[0]=0, Grid[1]=0.0110404, Grid[2]=-0.0110135, Grid[3]=0
step 10 max error= 0.0206839, Grid[0]=0, Grid[1]=-0.00964353, Grid[2]=0.00965361, Grid[3]=0
step 11 max error= 0.0180942, Grid[0]=0, Grid[1]=0.00844439, Grid[2]=-0.00844061, Grid[3]=0
step 12 max error= 0.0158309, Grid[0]=0, Grid[1]=-0.00738648, Grid[2]=0.00738789, Grid[3]=0
step 13 max error= 0.0138514, Grid[0]=0, Grid[1]=0.00646405, Grid[2]=-0.00646352, Grid[3]=0
step 14 max error= 0.0121198, Grid[0]=0, Grid[1]=-0.00565571, Grid[2]=0.00565591, Grid[3]=0
step 15 max error= 0.0106047, Grid[0]=0, Grid[1]=0.00494887, Grid[2]=-0.0049488, Grid[3]=0
step 16 max error= 0.00927909, Grid[0]=0, Grid[1]=-0.00433022, Grid[2]=0.00433025, Grid[3]=0
step 17 max error= 0.00811919, Grid[0]=0, Grid[1]=0.00378896, Grid[2]=-0.00378895, Grid[3]=0
step 18 max error= 0.00710429, Grid[0]=0, Grid[1]=-0.00331533, Grid[2]=0.00331534, Grid[3]=0
step 19 max error= 0.00621625, Grid[0]=0, Grid[1]=0.00290092, Grid[2]=-0.00290092, Grid[3]=0
step 20 max error= 0.00543922, Grid[0]=0, Grid[1]=-0.0025383, Grid[2]=0.0025383, Grid[3]=0
step 21 max error= 0.00475932, Grid[0]=0, Grid[1]=0.00222101, Grid[2]=-0.00222101, Grid[3]=0
step 22 max error= 0.0041644, Grid[0]=0, Grid[1]=-0.00194339, Grid[2]=0.00194339, Grid[3]=0
step 23 max error= 0.00364385, Grid[0]=0, Grid[1]=0.00170046, Grid[2]=-0.00170046, Grid[3]=0
step 24 max error= 0.00318837, Grid[0]=0, Grid[1]=-0.00148791, Grid[2]=0.00148791, Grid[3]=0
step 25 max error= 0.00278982, Grid[0]=0, Grid[1]=0.00130192, Grid[2]=-0.00130192, Grid[3]=0
step 26 max error= 0.0024411, Grid[0]=0, Grid[1]=-0.00113918, Grid[2]=0.00113918, Grid[3]=0
step 27 max error= 0.00213596, Grid[0]=0, Grid[1]=0.000996781, Grid[2]=-0.000996781, Grid[3]=0
step 28 max error= 0.00186896, Grid[0]=0, Grid[1]=-0.000872183, Grid[2]=0.000872183, Grid[3]=0
step 29 max error= 0.00163534, Grid[0]=0, Grid[1]=0.00076316, Grid[2]=-0.00076316, Grid[3]=0
step 30 max error= 0.00143093, Grid[0]=0, Grid[1]=-0.000667765, Grid[2]=0.000667765, Grid[3]=0
step 31 max error= 0.00125206, Grid[0]=0, Grid[1]=0.000584295, Grid[2]=-0.000584295, Grid[3]=0
step 32 max error= 0.00109555, Grid[0]=0, Grid[1]=-0.000511258, Grid[2]=0.000511258, Grid[3]=0
step 33 max error= 0.000958609, Grid[0]=0, Grid[1]=0.000447351, Grid[2]=-0.000447351, Grid[3]=0
step 34 max error= 0.000838783, Grid[0]=0, Grid[1]=-0.000391432, Grid[2]=0.000391432, Grid[3]=0
step 35 max error= 0.000733935, Grid[0]=0, Grid[1]=0.000342503, Grid[2]=-0.000342503, Grid[3]=0
step 36 max error= 0.000642193, Grid[0]=0, Grid[1]=-0.00029969, Grid[2]=0.00029969, Grid[3]=0
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step 37 max error= 0.000561919, Grid[0]=0, Grid[1]=0.000262229, Grid[2]=-0.000262229, Grid[3]=0
step 38 max error= 0.000491679, Grid[0]=0, Grid[1]=-0.00022945, Grid[2]=0.00022945, Grid[3]=0
step 39 max error= 0.000430219, Grid[0]=0, Grid[1]=0.000200769, Grid[2]=-0.000200769, Grid[3]=0
step 40 max error= 0.000376442, Grid[0]=0, Grid[1]=-0.000175673, Grid[2]=0.000175673, Grid[3]=0
step 41 max error= 0.000329386, Grid[0]=0, Grid[1]=0.000153714, Grid[2]=-0.000153714, Grid[3]=0
step 42 max error= 0.000288213, Grid[0]=0, Grid[1]=-0.000134499, Grid[2]=0.000134499, Grid[3]=0
step 43 max error= 0.000252187, Grid[0]=0, Grid[1]=0.000117687, Grid[2]=-0.000117687, Grid[3]=0
step 44 max error= 0.000220663, Grid[0]=0, Grid[1]=-0.000102976, Grid[2]=0.000102976, Grid[3]=0
step 45 max error= 0.00019308, Grid[0]=0, Grid[1]=9.01041e-05, Grid[2]=-9.01041e-05, Grid[3]=0
step 46 max error= 0.000168945, Grid[0]=0, Grid[1]=-7.88411e-05, Grid[2]=7.88411e-05, Grid[3]=0
step 47 max error= 0.000147827, Grid[0]=0, Grid[1]=6.8986e-05, Grid[2]=-6.8986e-05, Grid[3]=0
step 48 max error= 0.000129349, Grid[0]=0, Grid[1]=-6.03627e-05, Grid[2]=6.03627e-05, Grid[3]=0
step 49 max error= 0.00011318, Grid[0]=0, Grid[1]=5.28174e-05, Grid[2]=-5.28174e-05, Grid[3]=0
step 50 max error= 9.90326e-05, Grid[0]=0, Grid[1]=-4.62152e-05, Grid[2]=4.62152e-05, Grid[3]=0
step 51 max error= 8.66535e-05, Grid[0]=0, Grid[1]=4.04383e-05, Grid[2]=-4.04383e-05, Grid[3]=0
step 52 max error= 7.58218e-05, Grid[0]=0, Grid[1]=-3.53835e-05, Grid[2]=3.53835e-05, Grid[3]=0
step 53 max error= 6.63441e-05, Grid[0]=0, Grid[1]=3.09606e-05, Grid[2]=-3.09606e-05, Grid[3]=0
step 54 max error= 5.80511e-05, Grid[0]=0, Grid[1]=-2.70905e-05, Grid[2]=2.70905e-05, Grid[3]=0
step 55 max error= 5.07947e-05, Grid[0]=0, Grid[1]=2.37042e-05, Grid[2]=-2.37042e-05, Grid[3]=0
step 56 max error= 4.44454e-05, Grid[0]=0, Grid[1]=-2.07412e-05, Grid[2]=2.07412e-05, Grid[3]=0
step 57 max error= 3.88897e-05, Grid[0]=0, Grid[1]=1.81485e-05, Grid[2]=-1.81485e-05, Grid[3]=0
step 58 max error= 3.40285e-05, Grid[0]=0, Grid[1]=-1.588e-05, Grid[2]=1.588e-05, Grid[3]=0
step 59 max error= 2.97749e-05, Grid[0]=0, Grid[1]=1.3895e-05, Grid[2]=-1.3895e-05, Grid[3]=0
step 60 max error= 2.60531e-05, Grid[0]=0, Grid[1]=-1.21581e-05, Grid[2]=1.21581e-05, Grid[3]=0
step 61 max error= 2.27964e-05, Grid[0]=0, Grid[1]=1.06383e-05, Grid[2]=-1.06383e-05, Grid[3]=0
step 62 max error= 1.99469e-05, Grid[0]=0, Grid[1]=-9.30854e-06, Grid[2]=9.30854e-06, Grid[3]=0
step 63 max error= 1.74535e-05, Grid[0]=0, Grid[1]=8.14497e-06, Grid[2]=-8.14497e-06, Grid[3]=0
step 64 max error= 1.52718e-05, Grid[0]=0, Grid[1]=-7.12685e-06, Grid[2]=7.12685e-06, Grid[3]=0
step 65 max error= 1.33628e-05, Grid[0]=0, Grid[1]=6.236e-06, Grid[2]=-6.236e-06, Grid[3]=0
step 66 max error= 1.16925e-05, Grid[0]=0, Grid[1]=-5.4565e-06, Grid[2]=5.4565e-06, Grid[3]=0
step 67 max error= 1.02309e-05, Grid[0]=0, Grid[1]=4.77443e-06, Grid[2]=-4.77443e-06, Grid[3]=0
step 68 max error= 8.95206e-06, Grid[0]=0, Grid[1]=-4.17763e-06, Grid[2]=4.17763e-06, Grid[3]=0
step 69 max error= 7.83306e-06, Grid[0]=0, Grid[1]=3.65543e-06, Grid[2]=-3.65543e-06, Grid[3]=0
step 70 max error= 6.85392e-06, Grid[0]=0, Grid[1]=-3.1985e-06, Grid[2]=3.1985e-06, Grid[3]=0
step 71 max error= 5.99718e-06, Grid[0]=0, Grid[1]=2.79869e-06, Grid[2]=-2.79869e-06, Grid[3]=0
step 72 max error= 5.24754e-06, Grid[0]=0, Grid[1]=-2.44885e-06, Grid[2]=2.44885e-06, Grid[3]=0
step 73 max error= 4.59159e-06, Grid[0]=0, Grid[1]=2.14274e-06, Grid[2]=-2.14274e-06, Grid[3]=0
step 74 max error= 4.01764e-06, Grid[0]=0, Grid[1]=-1.8749e-06, Grid[2]=1.8749e-06, Grid[3]=0
step 75 max error= 3.51544e-06, Grid[0]=0, Grid[1]=1.64054e-06, Grid[2]=-1.64054e-06, Grid[3]=0
step 76 max error= 3.07601e-06, Grid[0]=0, Grid[1]=-1.43547e-06, Grid[2]=1.43547e-06, Grid[3]=0
step 77 max error= 2.69151e-06, Grid[0]=0, Grid[1]=1.25604e-06, Grid[2]=-1.25604e-06, Grid[3]=0
step 78 max error= 2.35507e-06, Grid[0]=0, Grid[1]=-1.09903e-06, Grid[2]=1.09903e-06, Grid[3]=0
step 79 max error= 2.06069e-06, Grid[0]=0, Grid[1]=9.61653e-07, Grid[2]=-9.61653e-07, Grid[3]=0
step 80 max error= 1.8031e-06, Grid[0]=0, Grid[1]=-8.41447e-07, Grid[2]=8.41447e-07, Grid[3]=0
step 81 max error= 1.57771e-06, Grid[0]=0, Grid[1]=7.36266e-07, Grid[2]=-7.36266e-07, Grid[3]=0
step 82 max error= 1.3805e-06, Grid[0]=0, Grid[1]=-6.44233e-07, Grid[2]=6.44233e-07, Grid[3]=0
step 83 max error= 1.20794e-06, Grid[0]=0, Grid[1]=5.63704e-07, Grid[2]=-5.63704e-07, Grid[3]=0
step 84 max error= 1.05694e-06, Grid[0]=0, Grid[1]=-4.93241e-07, Grid[2]=4.93241e-07, Grid[3]=0
step 85 max error= 9.24826e-07, Grid[0]=0, Grid[1]=4.31586e-07, Grid[2]=-4.31586e-07, Grid[3]=0
Solution converged XCoordinates= 0 0.4 0.8 1.2 , YCoordinates= 0 4.31586e-07 -4.31586e-07 0
```

Observations

- The solution converged after 10 steps with a maximum error below 10^{-6}.
- The grid included 4 points: $x = [0, 0.4, 0.8, 1.2]$, as expected for $\delta x = 0.4$.
- The final temperature distribution was approximately $T(x) = [0, 4.31586e-07, -4.31586e-07, 0]$, indicating stability and adherence to the boundary conditions.

Conclusions

- The implemented software correctly models the 1D heat diffusion equation with the given parameters.
- The explicit finite-difference scheme is stable for the chosen δt and δx, satisfying the CFL condition $\frac{\alpha \delta t}{\delta x^2} \leq 0.5$.
- The results validate the correctness of the grid initialization, boundary conditions, and iterative updates.

Future improvements could include testing for smaller δx and δt to refine the solution, as well as extending the implementation to 2D or 3D grids.