NUMERICAL SCHEME FOR HEAT EQUATION WITH FIRST BOUNDARY CONDITION ON SQUARE DOMAIN

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1. Numercial Schemes For Heat Equation With First Boundary Condition

In this report we consider the following problem:

$$u_t = \Delta u = u_{xx} + u_{yy}, u|_{\partial D \times (0,1]} = 0$$

Here $D = (0,1) \times (0,1)$ is a square domain on the plane.

If we give the initial condition $u(x,y,0) = \sin(\pi x)\sin(\pi y)$, this PDE can be easily solved with solution $u(x,y,t) = e^{-2\pi^2 t}\sin(\pi x)\sin(\pi y)$

1.1. Numerical Methods.

In this report we use several numerical methods to solve the PDE. We test the **explicit scheme, implicit scheme** and the **Crank-Nicolson Scheme**.

1.1.1. *Explicit Scheme.*

The forward explicit scheme can be simply written as

$$\frac{U_{j,k}^{m+1} - U_{j,k}^{m}}{h_t} = \frac{U_{j+1,k}^{m} - 2U_{j,k}^{m} + U_{j-1,k}^{m}}{h_x^2} + \frac{U_{j,k+1}^{m} - 2U_{j,k}^{m} + U_{j,k-1}^{m}}{h_y^2}$$

Equally

$$U_{j,k}^{m+1} = [1 - 2(\mu_x + \mu_y)]U_{j,k}^{m} + \mu_x(U_{j+1,k}^{m} + U_{j-1,k}^{m}) + \mu_y(U_{j,k+1}^{m} + U_{j,k-1}^{m})$$

Then the numerical error has the formula

$$e_{j,k}^{m+1} = [1 - 2(\mu_x + \mu_y)]e_{j,k}^{m} + \mu_x(e_{j+1,k}^{m} + e_{j-1,k}^{m}) + \mu_y(e_{j,k+1}^{m} + e_{j,k-1}^{m}) - T_{j,k}^{m}h_t$$

Here $T_{j,k}^m = Tu(x_j, y_k, t_m)$ is the local truncation error and it is easy to prove that $Tu(x,y,t) = \frac{1}{2}u_tth_t - \frac{1}{12}(u_{xxxx}(x,y,t)h_x^2 + u_{yyyy}(x,y,t)h_y^2) + O(h_t^2 + h_x^4 + h_y^4)$

Consider the maximal principle which can be formatted as following:

Theorem(Maximal Principle) For the finite difference scheme L_h defined as

$$L_h U_j = \sum_{i \in J\backslash\{j\}} c_{i,j}U_i - c_jU_j$$

satisfies

- $J_D \neq \emptyset$ and $J = J_\Omega \cup J_D$ is connected
- for every $j \in J_\Omega$ we have $c_j, c_{i,j} > 0$ and $c_j \geq \sum_{i\in D_{L_h}(j)} c_{i,j}$

Then

$$\max_{i\in J_\Omega} U_i \leq \max\{\max_{i\in J_D} U_i, 0\}$$

To satisfy the Maximal Principle we need $\mu_x + \mu_y \leq \frac{1}{2}$

Next we apply Fourier analysis method to analysis the stability of the scheme. Let the Fourier wave as

$$U_{j,k}^m = \lambda_\alpha^m e^{i(\alpha_x x_j + \alpha_y y_k)}, \alpha = (\alpha_x, \alpha_y)$$

Then $\lambda_\alpha = 1 - 4(\mu_x \sin^2 \frac{\alpha_x h_x}{2} + \mu_y \sin^2 \frac{\alpha_y h_y}{2})$

1.1.2. *Implicit scheme.* Here we consider the implicit scheme has the following formula which contains the Crank-Nicolson Scheme as a special case

$$\begin{aligned}\frac{U_{j,k}^{m+1} - U_{j,k}^m}{h_t} &= (1-\theta)(\frac{\delta_x^2}{h_x^2} + \frac{\delta_y^2}{h_y^2})U_{j,k}^m + \theta(\frac{\delta_x^2}{h_x^2} + \frac{\delta_y^2}{h_y^2})U_{j,k}^{m+1} \\ &= (1-\theta)(\frac{U_{j+1,k}^m - 2U_{j,k}^m + U_{j-1,k}^m}{h_x^2} + \frac{U_{j,k+1}^m - 2U_{j,k}^m + U_{j,k-1}^m}{h_y^2}) + \\ &\theta(\frac{U_{j+1,k}^{m+1} - 2U_{j,k}^{m+1} + U_{j-1,k}^{m+1}}{h_x^2} + \frac{U_{j,k+1}^{m+1} - 2U_{j,k}^{m+1} + U_{j,k-1}^{m+1}}{h_y^2})\end{aligned}$$

For the Fourier wave $U_{j,k}^m = \lambda_\alpha^m e^{i(\alpha_x x_j + \alpha_y y_k)}$, we have

$$\lambda_\alpha = \frac{1 - 4(1-\theta)(\mu_x \sin^2 \frac{\alpha_x h_x}{2} + \mu_y \sin^2 \frac{\alpha_y h_y}{2})}{1 + 4\theta(\mu_x \sin^2 \frac{\alpha_x h_x}{2} + \mu_y \sin^2 \frac{\alpha_y h_y}{2})}$$

In order to obtain the stability we need

$$2(\mu_x + \mu_y)(1 - 2\theta) \leq 1, 0 \leq \theta \leq \frac{1}{2}$$

Why Crank-Nicolson Scheme Choose $\theta = \frac{1}{2}$

The local truncation error can be proof to be $O(h_t^2 + h_x^2 + h_y^2)$ when $\theta = \frac{1}{2}$ and to be $O(h_t + h_x^2 + h_y^2)$ when θ is other value.

2. Numerical Linear Algebra Methods Used In Solving The Scheme

2.1. **Classical Iterative Methods:G-s and CG.** Analysis see in textbooks.

2.2. **Multi-grid.** Analysis see in appendix.(Which will be updated at later version)

3. Numerical Results

3.1. **Implement Details.** In the Crank-Nicolson Scheme test, we use the **gmres,pcg** in matlab with can transfer a function handler as the parameter.

3.2. **Performance of different schemes.** In this section, all of the results is using **pcg** in order to get fast and robust solutions:

Test	Space step	Time step	CN Scheme	Implicit Scheme	Explicit Scheme
1	1/512	1/50	2.44e-7	6.88e-5	1.39e56
2	1/512	1/500	2.40e-11	5.79e-7	NaN
3	1/512	1/5000	**3.97e-16**	5.674e-9	1.393e56
4	1/128	1/50	2.43e-7	6.88e-5	7.80e32
5	1/128	1/500	1.55e-11	5.81e-7	7.79e32
6	1/128	1/5000	1.04e-12	5.82e-9	7.79e32
7	1/32	1/50	2.28e-7	6.90e-5	2.71e201
8	1/32	1/500	1.32e-10	6.02e-7	5.23e8
9	1/32	1/5000	2.55e-10	8.20e-9	3.62e-9

Table 1. Error at time $t = 0.2$

3.3. **Time that different NLA methods take.** In this part we test several NLA methods in the implicit scheme and plot the result in the table below

Test	Space step	Time step	Cholesky	Multigrid	Gauss-Seidel
1	1/16	1/20	2.846	3.17	3.258
2	1/32	1/20	3.21	3.04	3.258
3	1/64	1/20	3.49	3.44	4.44
4	1/64	1/20	9.36	**4.33**	10.60

Table 2. CPU time of different NLA methods while calculating the solution at $t = 0.2$

3.4. **Some interesting observation.**

- Sometimes the pde solver may become faster if the time step becomes smaller. It seems that the iterative number will become bigger, but at the same time the algebra equation $(I - \Delta t\Delta)u_{t+1} = u_t$ becomes easier.
- Stupid methods is faster at easy situation.
- CN scheme is also faster than implicit scheme.

4. Readme

In this section, I will introduce the arrangement of my code. To show the demo, you can run the code in **runme.m**

4.1. Usage of the code.

To get the answer you can use the functions **CN_heat.m,explicit_heat.m,implicit_heat.m**

The choice of **Scheme_tool.method** have the following choices:

For Crank-Nicolson Scheme, Scheme_tool.method can choose

- gmres
- pcg
- cg

For Implicit Scheme, Scheme_tool.method can choose

- gs
- pcg
- cg
- gmres
- test
- multigrid
- chol

4.2. Arangement of the code.

Code in different paths is different usage:

- **matrix_func**: Numerical Linear Algebra functions and the code to calculate the matrix of laplace operator.
- **multigrid**: Functions for multigrid methods including restrict and lifting operator, V cycle and the multigrid method for heat equation.
- **op**:Some useful tools to change the grid to a vector
- **pde_func**: PDE solvers for heat equation and the true answer to test
- **plot_func**: To turn the PDE's solution to a video.
- **tool:** Two matlab classes to show the tol and max_int of different methods