计算物理学15春季

第四次作业解题报告

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1 Wave Function

1.1 推导过程

需要求解的波函数偏微分方程的形式为:

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0 \tag{1.1}$$

其中c是波速。将波动方程在求解区间上分割为$u_0, u_1, \ldots, u_N$的等距点，并采用周期性边界条件:

$$u_0 = u_N \tag{1.2}$$

这样偏微分方程就可以写成线性方程组的形式

$$u_j^{n+1} = u_j^n - \frac{c\Delta t}{\Delta x}(u_j^n - u_{j-1}^n), j = 0, 1, \ldots, N \tag{1.3}$$

取$r = \frac{c\Delta t}{\Delta x}$，将这一组方程写成矩阵乘法的形式:

$$\begin{bmatrix} u_0^{n+1} \\ u_1^{n+1} \\ \vdots \\ u_N^{n+1} \end{bmatrix} = \begin{bmatrix} 1-r & 0 & \ldots & r \\ r & 1-r & \ldots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \ldots & r & 1-r \end{bmatrix} \begin{bmatrix} u_0^n \\ u_1^n \\ \vdots \\ u_N^n \end{bmatrix} \tag{1.4}$$

1.2 程序求解

将上面的矩阵用MATLAB语言编写成求解程序:

```
% upwind.m, a function implements upwind scheme
function upwind(init, r)
                                % make a column vector
  u = init(:);
  N = size(u, 1);

                                % A matrix (sparse)
  A = spdiags(repmat([1-r r], N), [0 -1], N, N);
  A(1,N) = r;

  for j=1:10000
    plot(u);

                                % adjust axis
    a = axis;
    axis([0 N a(3) a(4)]);
    xlabel('x');
    ylabel('u');
    text(0.8*N, 0.8*(a(4)-a(3)+a(3)), sprintf('step: %d', j));

                                % update u vector
    u = A*u;

    pause(0.01);
  end
end
```

选取初始条件为正弦波函数，即调用上述函数的方法为:

```
upwind(sin([0:0.1:2*pi]), 0.4);
```

这是$r = 0.4$的情形。为了观察波函数的演化过程，将不同时间（$j = 1,21,41,\dots,101$）的波函数画在同一张图上，如图Figure 1.1。让$r = 1$和$r = 1.5$，画出不同情况下的波函数演化图，如图Figure 1.2、Figure 1.3。

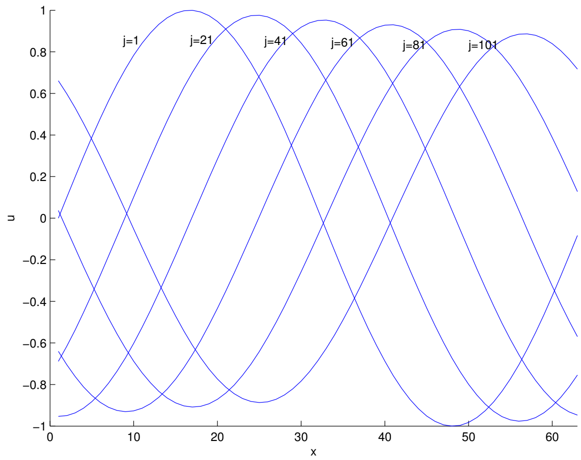
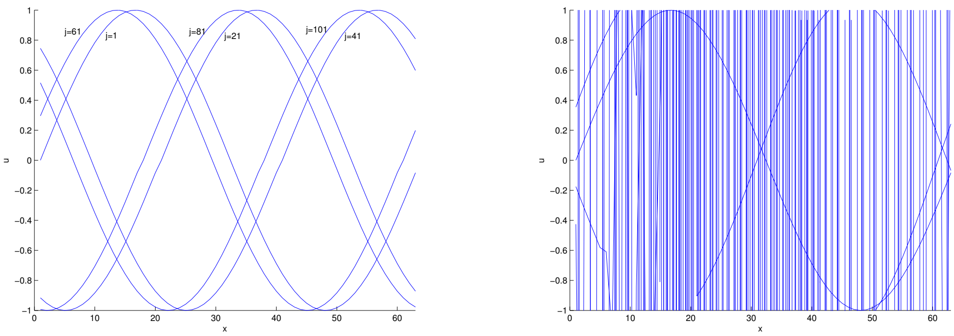


Figure 1.1: 波函数的演化，$r = 0.4$



(a) $r = 1.0$　　(b) $r = 1.5$

Figure 1.2: 不同r的求解

可以看到，Figure 1.1中，波函数的峰峰值不断下降，事实上我们的波动方程中并没有衰减项，矩阵解法的精度是有限的（采用有限步长近似实际上为方程加入了非线性项，导致解衰减）。其次可以发现r的选取对解的性质有很大的影响：如果r选择过大解就会发散；然而r的值和波速c有关，因此在不同的波速下需要选择不同的时间步长才能得到合适的解。

2 Boundary value problem

2.1 提出方程

y方向具有周期性边界条件，x方向有第一类边界条件的二维泊松方程写作：

$$\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=\rho(x,y), x\in[0,1], y\in[0,1] \tag{2.1}$$

$$u(x,0)=u(x,a) \tag{2.2}$$

$$u(0,y)=Y_0(y) \tag{2.3}$$

$$u(1,y)=Y_1(y) \tag{2.4}$$

将求解区域的x,y方向分别分割成N_x,N_y个点，在格点(i,j)处，泊松方程是：

$$\frac{2u(i,j)-u(i-1,j)-u(i+1,j)}{\Delta x^2}+\frac{2u(i,j)-u(i,j-1)-u(i,j+1)}{\Delta y^2}=\rho(i,j) \tag{2.5}$$

在y方向上进行傅立叶变换，并考虑到周期性边界条件$u(i,0)=u(i,N_y)$：

$$\sum_{j=1}^{N_y} e^{i\frac{2\pi}{N_y}k(j-1)}\rho(i,j)=g(i,k) \tag{2.6}$$

$$\sum_{j=1}^{N_y} e^{i\frac{2\pi}{N_y}k(j-1)}u(i,j)=f(i,k) \tag{2.7}$$

$$\sum_{j=1}^{N_y} e^{i\frac{2\pi}{N_y}k(j-1)}u(i,j-1)=e^{i\frac{2\pi}{N_y}k}f(i,k) \tag{2.8}$$

$$\sum_{j=1}^{N_y} e^{i\frac{2\pi}{N_y}k(j-1)}u(i,j+1)=e^{-i\frac{2\pi}{N_y}k}f(i,k) \tag{2.9}$$

x的左右边界同样通过傅立叶变换变换成序列$f_0(k)$和$f_1(k)$。根据上面三个式子，再结合之前的一维微分方程的矩阵解法，可以重新将二维泊松方程写成：

$$(\mathbf{A}-\frac{1}{\Delta y^2}4sin^2(\frac{\pi}{N_y}k)\mathbf{I})\begin{bmatrix} f(2,k)\\ f(3,k)\\ \vdots\\ f(N_x-1,k)\end{bmatrix}=\frac{1}{\Delta x^2}\begin{bmatrix} f_0(k)\\ 0\\ \vdots\\ f_1(k)\end{bmatrix}+\begin{bmatrix} g(2,k)\\ g(3,k)\\ \vdots\\ g(N_x-1,k)\end{bmatrix} \tag{2.10}$$

其中，

$$\mathbf{A} = \frac{1}{\Delta x^2}\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix} \tag{2.11}$$

根据上面的一维方程求出$u(i,k)$之后，再根据逆傅立叶变换求出泊松方程的解：

$$\frac{1}{N_y}\sum_{k=1}^{N_y} e^{-i\frac{2\pi}{N_y}j(k-1)} f(i,k) = u(i,j) \tag{2.12}$$

2.2 问题求解

使用MATLAB编写求解上述二维泊松方程的程序，如下：

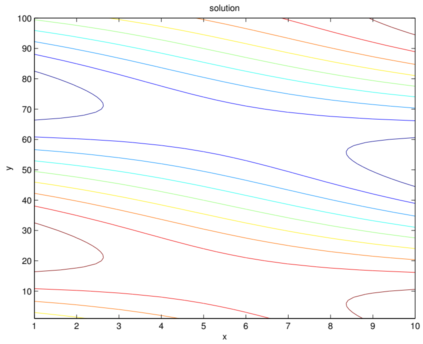
```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% function fourier_solve, a demonstration of
% solving possion PDE using fourier seris
%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function fourier_solve()
                 % x: left_border:0, right_border:1, source:1/(NX+1)->NX/(NX+1)
                 % y: source: 0->(NY-1)/NY
                 % dx=1/(NX+1), dy=1/NY
  NY = 100;
  NX = 10;

  dx = 1/(NX+1);
  dy = 1/NY;

                             % fill left/right border and source
  left = transpose(border_left_function([0:NY-1]*dy));
  right = transpose(border_right_function([0:NY-1]*dy));
  [mesh_x, mesh_y] = meshgrid([1:NX]*dx,[0:NY-1]*dy);
  source = source_function(mesh_x, mesh_y);

                             % transform them into fourier seris
  left_f = fourier(left);
  right_f = fourier(right);
  source_f = fourier(source);

                             % solve 1d problems under parameter k
  u = zeros(NY, NX);
```

```
  for j=1:NY
    u(j,:) = solve_1d(source_f(j,:), left_f(j), right_f(j), NX, NY, dx, dy,
        j-1);
  end

                              % transform back
  u = reverse_fourier(u);

  figure;
  imagesc(real(u));
  xlabel('x');
  ylabel('y');
  title('solution');
  colorbar;

  figure;
  imagesc(solution_function(mesh_x, mesh_y));
  xlabel('x');
  ylabel('y');
  title('original solution')
  colorbar;
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% test case
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function u=solution_function(x,y)
                              % test case 1
  % u = x.^2;

                              % test case 2
  % u = sin(2*pi*y);

                              % test case 3
  u = sin(2*pi*y).*(1-x)+ x.*cos(2*pi*y);
end
function u=border_left_function(y)
                              % test case 1
  % u = 0*y;

                              % test case 2
  % u = sin(2*pi*y);

                              % test case 3
  u = sin(2*pi*y);
end
function u=border_right_function(y)
                              % test case 1
  % u = 1 * ones(1, size(y(:), 1));
```

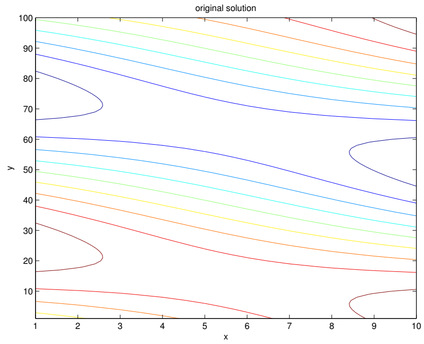
```
                               % test case 2
  % u = sin(2*pi*y);

                               % test case 3
  u = cos(2*pi*y);
end
function u=source_function(x,y)
                               % test case 1
  % u = ones(size(x,1),size(x,2));

                               % test case 2
  % u = -4*pi^2*sin(2*pi*y);

                               % test case 3
  u = -4*pi^2*(sin(2*pi*y).*(1-x)+ x.*cos(2*pi*y));
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% test case end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% solve 1d problem d^2u/dx^2 - 4sin(pi*k/NY)^2 u = rho(x)
%
% source: NX-by-1 matrix
% left: numeric, left border condition
% right: numeric, right border condition
% NX, NY: integer,
% dx: numeric
% k: numeric
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function u = solve_1d(source, left, right, NX, NY, dx, dy, k)
  A = spdiags(repmat([-1 2 -1], NX, 1), [1 0 -1], NX, NX) / dx^2;
  B = A - 4*(sin(pi/NY*k))^2 / dy^2 * eye(NX);

  b = zeros(NX, 1);
  b(1) = left / dx^2;
  b(NX) = right / dx^2;
  b = b + source(:);

  u = B \ b;
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% transform a list of vectors into its fourier seris
%
% input: N-by-M matrix of M vectors to transform
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function output=fourier(input)
```

```
  N = size(input, 1);

  A = ones(N);

  K = 2*pi/N;
  for j=1:N
    for k=1:N
      A(j,k) = exp((j-1)*(k-1)*i*K);
    end
  end

  output = zeros(size(input,1),size(input,2));
  for j=1:size(input,2)
    output(:,j) = A*input(:,j);
  end
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% transform a list of fourier seris back
%
% input: N-by-M matrix of M vectors to transform
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function output=reverse_fourier(input)
  N = size(input, 1);

  A = ones(N);

  K = 2*pi/N;
  for j=1:N
    for k=1:N
      A(j,k) = exp(-(j-1)*(k-1)*i*K) / N;
    end
  end

  output = zeros(size(input,1),size(input,2));
  for j=1:size(input,2)
    output(:,j) = A*input(:,j);
  end
end
```

上面的程序中，共提出了三种测试用的解析解，使用解为$u(x,y) = sin(2\pi y)(1-x) + xcos(2\pi y)$的测试用例求解结果如下（为了便于打印已将imagesc函数换成contour函数）：



(a) 程序求出的解



(b) 解析解

Figure 2.1: 二维泊松方程求解

2.3 遇到的问题

对复矩阵进行转置（transpose）的操作会求矩阵的转置后再取复共轭，这常常会导致不可预料的错误，因此应该使用下面的代码将行矩阵转换成列矩阵

```
m = m(:)
```

另外，为了避免不必要的计算，可以将傅立叶变换矩阵求出后存入静态变量。但是由于目前不是十分了解MATLAB编程语言，暂时没有找到合适的方法。
最后，选择测试用例的时候需要特别注意，测试用例的y方向上由于需要满足周期性边界条件，因此必须保证在端点处的函数值和导数连续，否则就无法求解。