

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Project Report

18.0851

COMPUTATIONAL SCIENCE AND ENGINEERING I

WRITTEN BY

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SUBMITTED TO:

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1 Problem Description

One-Dimensional Heat Equation

$$\frac{\partial u}{\partial t} = K \frac{\partial^2 u}{\partial x^2} + q(x, t) \quad (1)$$

Assumptions

1. Uniform Grid Spacing (Δx)
2. Uniform Time Steps (Δt)

Variables

Length of Domain: $L = 2 * \pi$

Left Boundary Condition: $C_1 = 1$

Right Boundary Condition: $C_2 = -0.2$

Thermal Diffusivity: $K = 0.1$

Boundary Conditions

Dirilecht Condition at the Left Boundary $x = 0$:

$$u(x = 0, t) = \begin{cases} C_1 * \frac{t}{t_{ramp}} & t \leq t_{ramp} \\ C_1 & t > t_{ramp} \end{cases} \quad (2)$$

Neumann Condition at the Right Boundary $x = L$:

$$\frac{\partial u}{\partial x}(x = L, t) = C_2 \quad (3)$$

Heating Source Function

$$q(x, t) = 0 \quad (4)$$

$$q(x, t) = -\sin(\omega t) * \exp\left(\frac{-(x - \frac{L}{2})^2}{\sigma^2}\right) \quad (5)$$

Second Order Finite Difference

At time t , where $u^{(n)} = \frac{\partial^n u}{\partial x^n}$

Taylor Expansions:

$$u(x + \Delta x) = u(x) + \Delta x u^{(1)}(x) + \frac{1}{2}(\Delta x)^2 u^{(2)}(x) + \frac{1}{6}(\Delta x)^3 u^{(3)}(x) + O(h^4) \quad (6)$$

$$u(x - \Delta x) = u(x) - \Delta x u^{(1)}(x) + \frac{1}{2}(\Delta x)^2 u^{(2)}(x) - \frac{1}{6}(\Delta x)^3 u^{(3)}(x) + O(h^4) \quad (7)$$

$$u(x + \Delta x) + u(x - \Delta x) = 2u(x) + (\Delta x)^2 u^{(2)}(x) + O(h^4) \quad (8)$$

Quadratic Convergence

$$u^{(2)}(x) = \frac{u(x + \Delta x) - 2u(x) + u(x - \Delta x)}{(\Delta x)^2} + O(h^2) \quad (9)$$

Explicit Euler
Implicit Euler
Crank-Nicolson

2 Appendix

MATLAB Code for Numerical Solution of Heat Equation

Listing 1: Numerical Heat Equation

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%% 18.0851 Project
% Author      : Jered Dominguez-Trujillo
% Date       : May 2, 2019
% Description : Numerical Solution to Heat Equation

% SCHEME = 0 -> EXPLICIT
% SCHEME = 1 -> IMPLICIT
% SCHEME = 2 -> CRANK_NICOLSON

function NumHT(SCHEME, BC1, BC2, KT, L, NX, TM, NT, TR, SOURCE_FLAG, W, SIGMA, QMAX)
    close all; clc;

    % Boundary Conditions
    LENGTH = L;                                % Length of Domain
    TIME_RAMP = TR;                             % Time Ramp at X = 0 for BC to Go from 0 to C1
    C1 = BC1;                                   % Dirilecht Condition U(x) = C1 at X = 0
    C2 = BC2;                                   % Neumann Condition at dU/dX = C2 at X = L
    K = KT;                                     % Thermal Diffusivity

    % Default Arguments
    if nargin <= 12
        QMAX = 1;                               % Default Maximum Value of Heat Source Function

        if nargin <= 11
            SIGMA = 0.2 * LENGTH;               % Default Standard Deviation of Heat Source Function
        end

        if nargin <= 10
            W = 1;                               % Default Frequency of Heat Source Function (rad/s)
        end
    end

    % Spatial Domain
    NODES = NX;                                % Nodes
    DX = LENGTH / NODES;                       % DX Calculation
    X = linspace(0, LENGTH + DX, NODES + 2); % X Vector with Ghost Node

    % Time Domain
    TMAX = TM;                                  % End Time of Simulation
    DT = TMAX / NT;                             % DT Calculation
    TIMESTEPS = TMAX / DT + 1;                 % Number of Time Steps
    T = linspace(0, TMAX, TIMESTEPS);          % Time Vector

    % Calculate CFL Number
    CFL = (DT .* K) ./ (DX .* DX);             % Multiplication Factor K (DT / DX^2)

    % Print Out Simulation Info
    if SCHEME == 0
        fprintf('Explicit Method:\n');
    elseif SCHEME == 1
        fprintf('Implicit Method:\n');
    elseif SCHEME == 2
        fprintf('Crank-Nicolson Method:\n');
    end

    fprintf('BCs:\n(1) U(x) = %.2f At X = 0\n(2) dU/dX = %.2f at X = L = %.2f\n\n', C1, C2, L);

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fprintf('Length: %.2f\t\tDX: %.2f\t\tNodes: %.0f\n', LENGTH, DX, NODES);
fprintf('Max Time: %.2f\t\tDT: %.2f\t\t\n', TMAX, DT);
if SOURCE_FLAG == 1
    fprintf('Q(x) = - QMAX * SIN(OMEGA * T) * EXP(-(X - L/2)^2 / SIGMA ^ 2)\n');
    fprintf('QMAX: %.2f\t\tOMEGA: %.2f rad/s\t\tSIGMA: %.2f\t\tL: %.2f\n', QMAX, W, SIGMA,
        LENGTH);
end
fprintf('CFL Number: %.2f\n', CFL);

% Initialize Matrices
U = zeros(TIMESTEPS, NODES + 2);
Q = zeros(TIMESTEPS, NODES + 2);

% If Heat Source Flag is True
if SOURCE_FLAG == 1
    for ii = 1:TIMESTEPS
        Q(ii, :) = - QMAX .* (sin((W .* T(ii)))) .* exp(-(X - (LENGTH ./ 2)) .^ 2) ./ (SIGMA .^
            2));
    end
end

% Initialize
CURRENT_T = 0;
TIMESTEP = 0;

% Plot Initial Conditions
fTemperature = figure('Name', 'Temperature History', 'NumberTitle', 'off');
figure(fTemperature);

% Temperature Profile
subplot(211);
plot(X, U(1, :), 'o-');
xlabel('X', 'FontSize', 18); ylabel('T', 'FontSize', 18);
axis([0 LENGTH -2 2]);

% Heat Source Profile
subplot(212);
plot(X, Q(1, :), 'o-');
xlabel('X', 'FontSize', 18); ylabel('Q', 'FontSize', 18);
axis([0 LENGTH -QMAX QMAX]);

suptitle(['Time = ', num2str(CURRENT_T), ' s']);
pause();

% Explicit Scheme
if SCHEME == 0

    % Iterate Until TMAX
    while CURRENT_T < TMAX
        CURRENT_T = CURRENT_T + DT;
        TIMESTEP = TIMESTEP + 1;

        n = TIMESTEP;

        % Explicit Euler Method
        for ii = 2:NODES + 1
            U(n + 1, ii) = CFL .* U(n, ii + 1) + (1 - 2 .* CFL) .* U(n, ii) + CFL .* U(n, ii -
                1) + Q(n, ii) .* DT;
        end

        % Boundary Conditions

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    U(n + 1, 1) = C1 * (CURRENT_T / TIME_RAMP) * (CURRENT_T <= TIME_RAMP) + C1 * (CURRENT_T
        > TIME_RAMP);
    U(n + 1, NODES + 2) = U(n + 1, NODES) + 2 * DX * C2;

    % Plot New Temperature Profile
    figure(fTemperature);

    % Temperature Profile
    subplot(211);
    plot(X, U(n + 1, :), 'o-');
    xlabel('X', 'FontSize', 18); ylabel('T', 'FontSize', 18);
    axis([0 L -2 2]);

    % Heat Source Profile
    subplot(212);
    plot(X, Q(n + 1, :), 'o-');
    xlabel('X', 'FontSize', 18); ylabel('Q', 'FontSize', 18);
    axis([0 LENGTH -QMAX QMAX]);

    suptitle(['Time = ', num2str(CURRENT_T), ' s']);

    pause(0.01);
end

% Implicit Scheme
elseif SCHEME == 1
    LOWER = zeros(1, NODES);
    DIAG = zeros(1, NODES + 1);
    UPPER = zeros(1, NODES);

    LOWERI = 2:NODES + 1; LOWERJ = 1:NODES;
    DIAGI = 1:NODES + 1; DIAGJ = 1:NODES + 1;
    UPPERI = 1:NODES; UPPERJ = 2:NODES + 1;

    DIAG(1) = 1; UPPER(1) = 0;

    for ii = 2:NODES
        LOWER(ii) = -CFL;
        DIAG(ii) = 2 * CFL + 1;
        UPPER(ii) = -CFL;
    end

    DIAG(NODES + 1) = 2 * CFL + 1;

    % Iterate Until TMAX
    while CURRENT_T < TMAX
        CURRENT_T = CURRENT_T + DT;
        TIMESTEP = TIMESTEP + 1;

        n = TIMESTEP;

        RHS = zeros(NODES + 1, 1);

        % Implicit Euler Method
        for ii = 2:NODES + 1
            RHS(ii) = U(n, ii) + Q(n, ii) .* DT;
        end

        % Boundary Conditions
        fBC1 = C1 * (CURRENT_T / TIME_RAMP) * (CURRENT_T <= TIME_RAMP) + C1 * (CURRENT_T >
            TIME_RAMP);
        LOWER(1) = 0;

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RHS(1) = fBC1;
RHS(2) = RHS(2) + CFL .* fBC1;

% Forward Difference Scheme
% DIAG(NODES + 1) = CFL + 1;
% RHS(NODES + 1) = RHS(NODES + 1) + C2 .* CFL .* DX;

% Central Difference Scheme
L(NODES) = -2 * CFL;
RHS(NODES + 1) = RHS(NODES + 1) + 2 .* C2 .* CFL .* DX;

MA = sparse([LOWERI, DIAGI, UPPERI], [LOWERJ, DIAGJ, UPPERJ], [LOWER, DIAG, UPPER],
            NODES + 1, NODES + 1);

U(n + 1, 1:end-1) = MA \ RHS;

% Forward Difference Scheme
% U(n + 1, end) = U(n + 1, end - 1) + C2 .* DX;

% Central Difference Scheme
U(n + 1, end) = U(n + 1, end - 2) + 2 .* C2 .* DX;

% Plot New Temperature Profile
figure(fTemperature);

% Temperature Profile
subplot(211);
plot(X, U(n + 1, :), 'o-');
xlabel('X', 'FontSize', 18); ylabel('T', 'FontSize', 18);
axis([0 LENGTH -0.5 1.5]);

% Heat Source Profile
subplot(212);
plot(X, Q(n + 1, :), 'o-');
xlabel('X', 'FontSize', 18); ylabel('Q', 'FontSize', 18);
axis([0 LENGTH -QMAX QMAX]);

suptitle(['Time = ', num2str(CURRENT_T), ' s']);

pause(0.01);
end

% Crank-Nicolson Scheme
elseif SCHEME == 2
    LOWER = zeros(1, NODES);
    DIAG = zeros(1, NODES + 1);
    UPPER = zeros(1, NODES);

    LOWERI = 2:NODES + 1; LOWERJ = 1:NODES;
    DIAGI = 1:NODES + 1; DIAGJ = 1:NODES + 1;
    UPPERI = 1:NODES; UPPERJ = 2:NODES + 1;

    DIAG(1) = 1; UPPER(1) = 0;

    for ii = 2:NODES
        LOWER(ii) = -CFL ./ 2;
        DIAG(ii) = CFL + 1;
        UPPER(ii) = -CFL ./ 2;
    end

    DIAG(NODES + 1) = CFL + 1;

```

```

% Iterate Until TMAX
while CURRENT_T < TMAX
    CURRENT_T = CURRENT_T + DT;
    TIMESTEP = TIMESTEP + 1;

    n = TIMESTEP;

    RHS = zeros(NODES + 1, 1);

    % Crank-Nicolson Method
    for ii = 2:NODES + 1
        RHS(ii) = CFL .* U(n, ii - 1) ./ 2 + (1 - CFL) .* U(n, ii) + CFL .* U(n, ii + 1) ./
            2 + Q(n, ii) .* DT;
    end

    % Boundary Conditions
    fBC1 = C1 * (CURRENT_T / TIME_RAMP) * (CURRENT_T <= TIME_RAMP) + C1 * (CURRENT_T >
        TIME_RAMP);
    LOWER(1) = 0;
    RHS(1) = fBC1;
    RHS(2) = RHS(2) + CFL .* fBC1 ./ 2;

    % Forward Difference Scheme
    % DIAG(NODES + 1) = CFL ./ 2 + 1;
    % RHS(NODES + 1) = RHS(NODES + 1) + C2 .* CFL .* DX ./ 2;

    % Central Difference Scheme
    L(NODES) = -CFL;
    RHS(NODES + 1) = RHS(NODES + 1) + C2 .* CFL .* DX;

    MA = sparse([LOWERI, DIAGI, UPPERI], [LOWERJ, DIAGJ, UPPERJ], [LOWER, DIAG, UPPER],
        NODES + 1, NODES + 1);

    U(n + 1, 1:end-1) = MA \ RHS;

    % Forward Difference Scheme
    % U(n + 1, end) = U(n + 1, end - 1) + C2 .* DX;

    % Central Difference Scheme
    U(n + 1, end) = U(n + 1, end - 2) + 2 .* C2 .* DX;

    % Plot New Temperature Profile
    figure(fTemperature);

    % Temperature Profile
    subplot(211);
    plot(X, U(n + 1, :), 'o-');
    xlabel('X', 'FontSize', 18); ylabel('T', 'FontSize', 18);
    axis([0 LENGTH -0.5 1.5]);

    % Heat Source Profile
    subplot(212);
    plot(X, Q(n + 1, :), 'o-');
    xlabel('X', 'FontSize', 18); ylabel('Q', 'FontSize', 18);
    axis([0 LENGTH -QMAX QMAX]);

    suptitle(['Time = ', num2str(CURRENT_T), ' s']);

    pause(0.01);
end
end
end

```