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SUBJECT: Method of Weighted Residuals – Collocation method

The purpose of this assignment is to learn about collocation method. A method that finds solutions for ordinary differential equations, partial differential equations and integral equations.

Introduction

The conservation balance of a species that diffuses and reacts is a partial differential equation, as shown in equation 1:

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r} - \phi^2 c \quad (1)$$

Where c is concentration, t is time, r is radial coordinate and ϕ is the Thiele modulus. This equation will be used throughout this assignment to solve for the unknown concentrations by using Lagrange polynomials with collocation. The concentrations were found using the "\" command and plotted. The residuals and analytical solution were also plotted.

Method

Part 1a:

Equation 1 was solved for in steady state with the following boundary conditions, equation (3), using Lagrangian polynomials as shown in equation (4):

$$\frac{\partial^2 c(r)}{\partial r^2} + \frac{1}{r}\frac{\partial c(r)}{\partial r} - \phi^2 c(r) = 0 \quad (2)$$

$$\frac{\partial c(r)}{\partial r} = 0,\ c(1) = 1 \quad (3)$$

$$\hat{c}(r) = \sum_{i=1}^{N} c_i l_i\,(r) \quad (4)$$

Four nodal points were chosen: 0, 0.25, 0.75, and 1. The nodal points were using to find the Lagrangian polynomials by hand. Once found, the first and second derivatives of the polynomials were found.

Part 1b:

The polynomials found in part 1a was expressed in the form of equation 1 for each node as vectors.

Part 1c:

The system of equations from part 1b were put in standard matrix form, Ax=b, with the vectors in part 1b being matrix A, the unknown concentrations being vector x, and vector [0 0 0 1] as vector b to comply with the boundary conditions in equation 3.

Part 1d:

The unknown concentrations were found in MATLAB by using the A\b and phi = 2. This multiplies the b vector by the inverse of the A matrix.

Part 2:

The concentration profile was plotted using the scatter function for the points and the plot function to connect the points. The points being the concentration at each node.

Part 3:

The residuals were plotted using the residual equation, equation 5, for the collocation method with phi=2:

$$R(\hat{c}, r) = \frac{\partial^2 \hat{c}}{\partial r^2} + \frac{1}{r}\frac{\partial \hat{c}}{\partial r} - \phi^2 \hat{c} \quad (5)$$

The residual error was plotted using the scatter function for the points and the plot function to connect the points. The points being the residual error at each node.

Part 4:

The analytical solution, shown in equation 6, was found using the Bessel function in MATLAB:

$$c(r) = \frac{I_0(\phi r)}{I_0(\phi)} \quad (6)$$

$$I_0(x) = \sum_{k=0}^{inf} \frac{\left(\frac{x}{2}^{2k}\right)}{k!\Gamma(k+1)} \quad (7)$$

The solution was plotted against an interval of 0 to 1 with 0.1 spacing using the plot function.

Results

Part 1a and 1b:

The Lagrangian polynomials and the derivatives of the polynomials were done by hand on a separate piece of paper.

Part 1c:

The vectors were arranged in standard matrix form in MATLAB in the following format:

$$\begin{bmatrix} l_0'(x_0) & l_1'(x_0) & l_2'(x_0) & l_3'(x_0) \\ l_0''(x_1) + \frac{1}{x_1} l_0'(x_1) - \phi^2 l_0(x_1) & l_1''(x_1) + \frac{1}{x_1} l_1'(x_1) - \phi^2 l_1(x_1) & l_2''(x_1) + \frac{1}{x_1} l_2'(x_1) - \phi^2 l_2(x_1) & l_3''(x_1) + \frac{1}{x_1} l_3'(x_1) - \phi^2 l_3(x_1) \\ l_0''(x_2) + \frac{1}{x_1} l_0'(x_2) - \phi^2 l_0(x_2) & l_1''(x_2) + \frac{1}{x_1} l_1'(x_2) - \phi^2 l_1(x_2) & l_2''(x_2) + \frac{1}{x_1} l_2'(x_2) - \phi^2 l_2(x_2) & l_3''(x_2) + \frac{1}{x_1} l_3'(x_2) - \phi^2 l_3(x_2) \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Part 1d:

The concentrations were found to be $x = \begin{bmatrix} 0.4373 \\ 0.4616 \\ 0.7213 \\ 1 \end{bmatrix}$

Part 2:

The concentration profile is shown below:

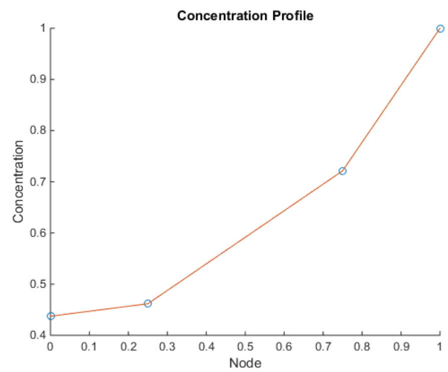

Figure 1 Concentration profile

Part 3:

The residuals for the collocation method are shown in the graph below:

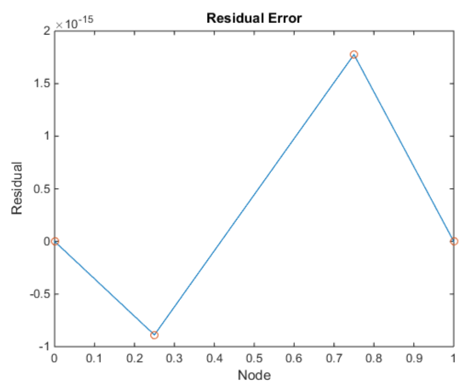

Figure 2 Residual error

Part 4:

The analytical solution was plotted and shown below:

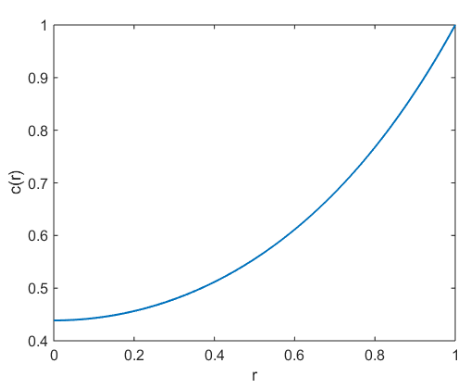

Figure 3 Analytical solution

Conclusion

The collocation method used Lagrangian polynomials to solve for the conservation balance of species equation to find the unknown concentrations. Using the standard matric form, which has been seen many times, and the knowledge obtained from solving for system of equations, we were able to find the unknown con entrations.

Discussion

The collocation method is good for solving for partial differential functions, just like equation 1. This assignment was effective in teaching how the collocation method works.

Appendix A

```
clc
clear all
close all

%Problem 1
x0 = 0;
x1 = .25;
x2 = .75;
x3 = 1;
phi = 2;

%L(x)
x=x0;
L0x0 = ((x^3)-(2*(x^2))+(1.1875*x)-0.1875)/(-0.1875);
L1x0 = ((x^3)-(1.75*(x^2))+(0.75*x))/0.09375;
L2x0 = ((x^3)-(1.25*(x^2))+(0.25*x))/(-0.09375);
L3x0 = ((x^3)-(x^2)+(0.1875*x))/0.1875;

x=x1;
L0x1 = ((x^3)-(2*(x^2))+(1.1875*x)-0.1875)/(-0.1875);
L1x1 = ((x^3)-(1.75*(x^2))+(0.75*x))/0.09375;
L2x1 = ((x^3)-(1.25*(x^2))+(0.25*x))/(-0.09375);
L3x1 = ((x^3)-(x^2)+(0.1875*x))/0.1875;

x=x2;
L0x2 = ((x^3)-(2*(x^2))+(1.1875*x)-0.1875)/(-0.1875);
L1x2 = ((x^3)-(1.75*(x^2))+(0.75*x))/0.09375;
L2x2 = ((x^3)-(1.25*(x^2))+(0.25*x))/(-0.09375);
L3x2 = ((x^3)-(x^2)+(0.1875*x))/0.1875;

x=x3;
L0x3 = ((x^3)-(2*(x^2))+(1.1875*x)-0.1875)/(-0.1875);
L1x3 = ((x^3)-(1.75*(x^2))+(0.75*x))/0.09375;
L2x3 = ((x^3)-(1.25*(x^2))+(0.25*x))/(-0.09375);
L3x3 = ((x^3)-(x^2)+(0.1875*x))/0.1875;

%L(x) derivative
x=x0;
L0Dx0 = ((3*(x^2))-(4*x)+1.1875)/(-0.1875);
L1Dx0 = ((3*(x^2))-(3.5*x)+0.75)/0.09375;
L2Dx0 = ((3*(x^2))-(2.5*x)+0.25)/(-0.09375);
L3Dx0 = ((3*(x^2))-(2*x)+0.1875)/0.1875;

x=x1;
L0Dx1 = ((3*(x^2))-(4*x)+1.1875)/(-0.1875);
L1Dx1 = ((3*(x^2))-(3.5*x)+0.75)/0.09375;
L2Dx1 = ((3*(x^2))-(2.5*x)+0.25)/(-0.09375);
L3Dx1 = ((3*(x^2))-(2*x)+0.1875)/0.1875;

x=x2;
L0Dx2 = ((3*(x^2))-(4*x)+1.1875)/(-0.1875);
L1Dx2 = ((3*(x^2))-(3.5*x)+0.75)/0.09375;
L2Dx2 = ((3*(x^2))-(2.5*x)+0.25)/(-0.09375);
L3Dx2 = ((3*(x^2))-(2*x)+0.1875)/0.1875;
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```
x=x3;
L0Dx3 = ((3*(x^2))-(4*x)+1.1875)/(-0.1875);
L1Dx3 = ((3*(x^2))-(3.5*x)+0.75)/0.09375;
L2Dx3 = ((3*(x^2))-(2.5*x)+0.25)/(-0.09375);
L3Dx3 = ((3*(x^2))-(2*x)+0.1875)/0.1875;

%L(x) Double Derivative
x=x0;
L0DDx0 = ((6*x)-4)/(-0.1875);
L1DDx0 = ((6*x)-3.5)/(0.09375);
L2DDx0 = ((6*x)-2.5)/(-0.09375);
L3DDx0 = ((6*x)-2)/0.1875;

x=x1;
L0DDx1 = ((6*x)-4)/(-0.1875);
L1DDx1 = ((6*x)-3.5)/(0.09375);
L2DDx1 = ((6*x)-2.5)/(-0.09375);
L3DDx1 = ((6*x)-2)/0.1875;

x=x2;
L0DDx2 = ((6*x)-4)/(-0.1875);
L1DDx2 = ((6*x)-3.5)/(0.09375);
L2DDx2 = ((6*x)-2.5)/(-0.09375);
L3DDx2 = ((6*x)-2)/0.1875;

x=x3;
L0DDx3 = ((6*x)-4)/(-0.1875);
L1DDx3 = ((6*x)-3.5)/(0.09375);
L2DDx3 = ((6*x)-2.5)/(-0.09375);
L3DDx3 = ((6*x)-2)/0.1875;

%at x1
c0x1 = L0DDx1 + ((1/x1)*L0Dx1);
c1x1 = L1DDx1 + ((1/x1)*L1Dx1)-((phi^2)*L1x1);
c2x1 = L2DDx1 + ((1/x1)*L2Dx1);
c3x1 = L3DDx1 + ((1/x1)*L3Dx1);

%at x2
c0x2 = L0DDx2 + ((1/x2)*L0Dx2);
c1x2 = L1DDx2 + ((1/x2)*L1Dx2);
c2x2 = L2DDx2 + ((1/x2)*L2Dx2)-((phi^2)*L2x2);
c3x2 = L3DDx2 + ((1/x2)*L3Dx2);

C0 = [L0Dx0 L1Dx0 L2Dx0 L3Dx0];
C1 = [c0x1 c1x1 c2x1 c3x1];
C2 = [c0x2 c1x2 c2x2 c3x2];
C3 = [0 0 0 1];

A = [C0;C1;C2;C3];
b = [0;0;0;1];
conc = A\b;

%Problem 2
int = [0;0.25;0.75;1];
```

```
scatter(int,conc)
hold on
plot(int,conc)
title('Concentration Profile');
xlabel('Node')
ylabel('Concentration')

%Problem 3
r = A*conc-b;
figure
plot(int,r)
hold on
scatter(int,r)
title('Residual Error')
xlabel('Node')
ylabel('Residual')

%Problem 4
int = (0:0.01:1).';
CAnalytical = besseli(0,phi*int)/besseli(0,phi);
figure;
plot(int,CAnalytical,'linewidth',1.5)
xlabel('r')
ylabel('c(r)')
set(gca,'fontsize',12)
```