Problem Set #10

Boundary Value Problem

1. Consider the following linear BVP

$$y'' - 3y' + 2y = x, \quad y(0) = 1, \quad y'(1) = 2$$

(a) Formulate the above BVP in order to solve numerically by shooting method.

(b) Using central difference approximation for the differential equation, develop the finite difference formulation that you intend to use in solving the above BVP numerically. Take h = 0.1.

Solution:

(a) $$y'' - 3y' + 2y = x, \quad y(0) = 1, \quad y'(1) = 2$$

Let	$y' = z$	$y(0) = 1$
then	$z' = x + 3z - 2y$	$y'(1) = z(1) = 2$

We can solve the above two first-order equations as initial value problem (IVP), if we know z at x = 0 instead of z at x = 1.

In the shooting method, we will guess z at x = 0, and will solve the resulting IVPs using Euler or RK4 and will match the value of z at x = 1 to see whether it is 2.

z (0)	z (1)
0.1	-6.6593
0.5	-1.8453
0.818	2

Since the differential equation is linear, we can determine the exact value of z(0) from the first two runs as follows

$$\text{Exact } z(0) = 0.1 + [(0.5 - 0.1) / (-1.8453 + 6.6593)]\,[2 + 6.6593] = 0.818$$

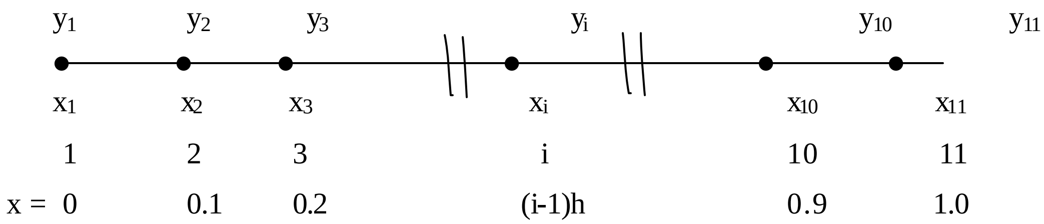
Therefore, exact solution of the differential equation can be obtained by solving the following equations

$y' = z$	$y(0) = 1$
$z' = x + 3z - 2y$	$z(0) = 0.818$

using Euler or RK4. The result will satisfy the boundary condition y'(1) = 2.

(b) Since $h = 0.1$, $n = (b - a)/h + 1 = (1 - 0)/0.1 + 1 = 11$

$x_i = a + (i - 1)h = (i - 1)h$



$$y'' - 3y' + 2y = x, \quad y(0) = 1, \quad y'(1) = 2$$

Therefore, $y(0) = y_1 = 1$ and $y'(1) = y_{11}' = 2$

We have 10 Unknowns: $y_2, y_3, y_4, y_5, y_6, y_7, y_8, y_9, y_{10}, y_{11}$

Note that y_1 is known but y_{11} is unknown.

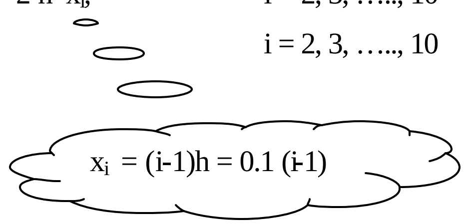
Discretization of the differential equation at general internal node (grid) i is given by

$$\left[\frac{y_{i-1} - 2y_i + y_{i+1}}{h^2}\right] - 3\left[\frac{y_{i+1} - y_{i-1}}{2h}\right] + 2y_i = x_i, \qquad i = 2, 3, \ldots, 10$$

Multiplying both sides by $2h^2$, and rearranging we have

$$[2 + 3h]\, y_{i-1} + 4[h^2 - 1]\, y_i + [2 - 3h]\, y_{i+1} = 2h^2 x_i, \qquad i = 2, 3, \ldots, 10$$

or, $$2.3\, y_{i-1} - 3.96\, y_i + 1.7\, y_{i+1} = 0.002\,(i-1), \qquad i = 2, 3, \ldots, 10$$



i = 2: $2.3\, y_1 - 3.96\, y_2 + 1.7\, y_3 = 0.002$

or, $-3.96\, y_2 + 1.7\, y_3 = 0.002 - 2.3\, y_1$

or, $-3.96\, y_2 + 1.7\, y_3 = -2.298$

i = 3: $2.3\, y_2 - 3.96\, y_3 + 1.7\, y_4 = 0.004$

i = 4: $2.3\, y_3 - 3.96\, y_4 + 1.7\, y_5 = 0.006$

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i = 9: $2.3\, y_8 - 3.96\, y_9 + 1.7\, y_{10} = 0.016$

i = 10: $2.3\, y_9 - 3.96\, y_{10} + 1.7\, y_{11} = 0.018$

At node 11, we have to apply the boundary condition. That is, $y_{11}' = 2$

If we use backward different approximation for y_{11}', we have

$$y_{11}' = \left[\frac{y_{11} - y_{10}}{h}\right] = 2 \quad \Rightarrow \quad -y_{10} + y_{11} = 2h = 0.2$$

Therefore, the matrix looks like

$$\begin{bmatrix} -3.96 & 1.7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2.3 & -3.96 & 1.7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2.3 & -3.96 & 1.7 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2.3 & -3.96 & 1.7 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.3 & -3.96 & 1.7 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2.3 & -3.96 & 1.7 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2.3 & -3.96 & 1.7 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2.3 & -3.96 & 1.7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2.3 & -3.96 & 1.7 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

Note that Matrix is
- Tri-diagonal
- Diagonally dominant
- Independent of y_i's

$$\times \begin{bmatrix} y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \\ y_{10} \\ y_{11} \end{bmatrix} = \begin{bmatrix} -2.298 \\ 0.004 \\ 0.006 \\ 0.008 \\ 0.010 \\ 0.012 \\ 0.014 \\ 0.016 \\ 0.018 \\ 0.2 \end{bmatrix}$$

Solving the above tri-diagonal matrix we can determine the values of y_2 to y_{11}.

Note that since the differential equation is linear, we obtained linear algebraic equations.

2. Consider the non-linear BVP

$$-\frac{d^2u}{dx^2} + u^3 = x^3, \quad 0 < x < 1$$

$$u'(0) = 0, \; u'(1) = 1$$

(a) Formulate the above BVP in order to solve numerically by shooting method.

(b) Using central difference approximation for the differential equation, develop the finite difference formulation that you intend to use in solving the above BVP numerically.

(i) State the equation in the form $\mathbf{f}_i(\mathbf{u}_i) = 0$ for the general i^{th} (interior) node.

(ii) State the equation in the form $f_1(\mathbf{u}_i) = 0$ for the 1^{st} boundary (at x = 0) node.

(iii) State the equation in the form $f_n(\mathbf{u}_i) = 0$ for the n^{th} boundary (at x = 1) node.

(iv) What is the bandwidth of the associated Jocobian for n = 100?

(v) Approximately, how accurate is u_i if n = 200 is used as compared to n = 100?

(vi) Divergence occurs in an attempted Newton-Raphson iteration solution to the above BVP for n = 100 and a particular initial guess. What can be concluded?

<u>Solution</u>:

$$-u'' + u^3 = x^3 \qquad u'(0) = 0, \; u'(1) = 1$$

Note that the differential equation is non-linear. It is non-linear because of the term u^3 and not because of the terms u'' or x^3.

(a) Let $u' = v$ $\qquad$ u(0) = Guess a value

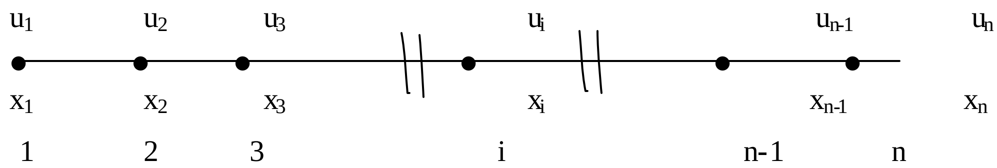
then $v' = u^3 - x^3$, $\qquad$ v(0) = 0, v(1) = 1

To apply the shooting method, we have to guess u(0) and solve using Euler, RK4 or other methods, and check whether v at x =1 is 1. Since the differential equation is non-linear, we will not be able to use linear interpolation to guess the correct value for u(0). We have to determine u(0) by repeated trial-and-error to match v(1) = 1.

Guess u(0)	v(1)	Guess u(0)	v(1)
0.1	-0.2492	1.0	1.5552
0.5	-0.1147	0.85	0.6529
0.8	0.4616	0.91	0.9439

1.5	24.36	**0.92**	**1.0001**

(b) $-u'' + u^3 = x^3$ $\quad$ $u'(0) = 0,\ u'(1) = 1$



Note that since both boundary conditions are derivative boundary conditions, we have n unknowns, u_1 to u_n, where n is the number of nodes or grid points.

(i) $$-\left[\frac{u_{i-1}-2u_i+u_{i+1}}{h^2}\right]+u_i^3 = x_i^3$$

or, $$f_i = u_{i-1} - [2 + h^2 u_i^2]\, u_i + u_{i+1} + h^2 x_i^3 = 0 \qquad i = 2, 3, \ldots, (n-1)$$

Note that since the differential equation is non-linear, the discretized equation is systems of non-linear algebraic equation.

(ii) At grid point 1, $u_1' = 0$.

That is, if we use forward difference approximation, we have at grid 1

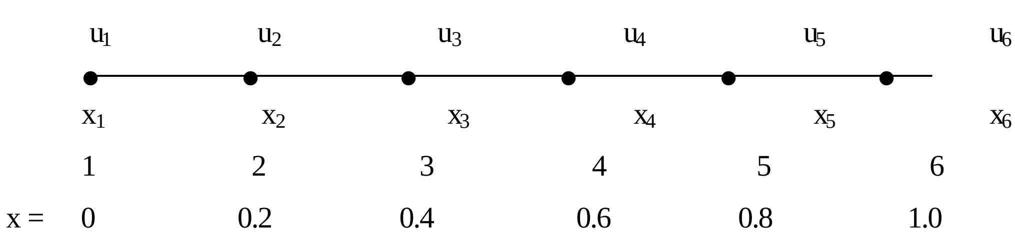
$$\left[\frac{u_2-u_1}{h}\right]=0 \quad \Rightarrow \quad f_1 = u_1 - u_2 = 0$$

(iii) At grid point n, $u_n' = 1$.

That is, if we use backward difference approximation, we have at grid n

$$\left[\frac{u_n-u_{n-1}}{h}\right]=1 \quad \Rightarrow \quad f_n = u_n - u_{n-1} - h = 0$$

(iv) Let us assume n = 6 (total of 6 grid (node) points). Then, we have



We have 6 unknowns, u_1, u_2, u_3, u_4, u_5, and u_6.

The 6 non-linear equations are given by

$f_1 = u_1 - u_2 = 0$ — Boundary point

$f_2 = u_1 - [2 + h^2 u_2^2]\, u_2 + u_3 + h^2 x_2^3 = 0$

$f_3 = u_2 - [2 + h^2 u_3^2]\, u_3 + u_4 + h^2 x_3^3 = 0$ — Interior point

$f_4 = u_3 - [2 + h^2 u_4^2]\, u_4 + u_5 + h^2 x_4^3 = 0$

$f_5 = u_4 - [2 + h^2 u_5^2]\, u_5 + u_6 + h^2 x_5^3 = 0$

$f_6 = u_6 - u_5 - h = 0$ — Boundary point

The 6 unknowns need to be determined from the above 6 non-linear equations. We have to use Newton-Raphson's method to solve the 6 unknowns from the 6 non-linear equations. We have to solve

$$\mathbf{J}\ \Delta\mathbf{u} = -\boldsymbol{f}$$

$$\begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} & \frac{\partial f_1}{\partial u_3} & \frac{\partial f_1}{\partial u_4} & \frac{\partial f_1}{\partial u_5} & \frac{\partial f_1}{\partial u_6} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} & \frac{\partial f_2}{\partial u_3} & \frac{\partial f_2}{\partial u_4} & \frac{\partial f_2}{\partial u_5} & \frac{\partial f_2}{\partial u_6} \\ \frac{\partial f_3}{\partial u_1} & \frac{\partial f_3}{\partial u_2} & \frac{\partial f_3}{\partial u_3} & \frac{\partial f_3}{\partial u_4} & \frac{\partial f_3}{\partial u_5} & \frac{\partial f_3}{\partial u_6} \\ \frac{\partial f_4}{\partial u_1} & \frac{\partial f_4}{\partial u_2} & \frac{\partial f_4}{\partial u_3} & \frac{\partial f_4}{\partial u_4} & \frac{\partial f_4}{\partial u_5} & \frac{\partial f_4}{\partial u_6} \\ \frac{\partial f_5}{\partial u_1} & \frac{\partial f_5}{\partial u_2} & \frac{\partial f_5}{\partial u_3} & \frac{\partial f_5}{\partial u_4} & \frac{\partial f_5}{\partial u_5} & \frac{\partial f_5}{\partial u_6} \\ \frac{\partial f_6}{\partial u_1} & \frac{\partial f_6}{\partial u_2} & \frac{\partial f_6}{\partial u_3} & \frac{\partial f_6}{\partial u_4} & \frac{\partial f_6}{\partial u_5} & \frac{\partial f_6}{\partial u_6} \end{bmatrix} \begin{bmatrix} u_1^{(k+1)} - u_1^{(k)} \\ u_2^{(k+1)} - u_2^{(k)} \\ u_3^{(k+1)} - u_3^{(k)} \\ u_4^{(k+1)} - u_4^{(k)} \\ u_5^{(k+1)} - u_5^{(k)} \\ u_6^{(k+1)} - u_6^{(k)} \end{bmatrix} = -\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}$$

$f_1 = u_1 - u_2 = 0$

$$\frac{\partial f_1}{\partial u_1} = 1,\ \ \frac{\partial f_1}{\partial u_2} = -1,\ \ \frac{\partial f_1}{\partial u_i} = 0 \quad \text{for i = 3, 4, 5, 6.}$$

$f_2 = u_1 - [2 + h^2 u_2^2]\, u_2 + u_3 + h^2 x_2^3 = 0$

$$\frac{\partial f_2}{\partial u_1} = 1,\ \ \frac{\partial f_2}{\partial u_2} = -\left(2 + 3h^2 u_2^2\right),\ \ \frac{\partial f_2}{\partial u_3} = 1,\ \ \frac{\partial f_2}{\partial u_i} = 0 \quad \text{for i = 4, 5, 6.}$$

$f_3 = u_2 - [2 + h^2 u_3^2]\, u_3 + u_4 + h^2 x_3^3 = 0$

$$\frac{\partial f_3}{\partial u_2} = 1,\ \ \frac{\partial f_3}{\partial u_3} = -\left(2 + 3h^2 u_3^2\right),\ \ \frac{\partial f_3}{\partial u_4} = 1,\ \ \frac{\partial f_3}{\partial u_i} = 0 \quad \text{for i = 1, 5, 6.}$$

$f_4 = u_3 - [2 + h^2 u_4^2]\, u_4 + u_5 + h^2 x_4^3 = 0$

$$\frac{\partial f_4}{\partial u_3} = 1, \quad \frac{\partial f_4}{\partial u_4} = -\left(2 + 3h^2 u_4^2\right), \quad \frac{\partial f_4}{\partial u_5} = 1, \quad \frac{\partial f_4}{\partial u_i} = 0 \quad \text{for i = 1, 2, 6.}$$

$f_5 = u_4 - [2 + h^2 u_5^2]\, u_5 + u_6 + h^2 x_5^3 = 0$

$$\frac{\partial f_5}{\partial u_4} = 1, \quad \frac{\partial f_5}{\partial u_5} = -\left(2 + 3h^2 u_5^2\right), \quad \frac{\partial f_5}{\partial u_6} = 1, \quad \frac{\partial f_5}{\partial u_i} = 0 \quad \text{for i = 1, 2, 3.}$$

$f_6 = u_6 - u_5 - h = 0$

$$\frac{\partial f_6}{\partial u_5} = -1, \quad \frac{\partial f_6}{\partial u_6} = 1, \quad \frac{\partial f_6}{\partial u_i} = 0 \quad \text{for i = 1, 2, 3, 4.}$$

Therefore, we have

$$\begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ 1 & -(2+0.12\,u_2^2) & 1 & 0 & 0 & 0 \\ 0 & 1 & -(2+0.12\,u_3^2) & 1 & 0 & 0 \\ 0 & 0 & 1 & -(2+0.12\,u_4^2) & 1 & 0 \\ 0 & 0 & 0 & 1 & -(2+0.12\,u_5^2) & 1 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} \Delta u_1^{(k)} \\ \Delta u_2^{(k)} \\ \Delta u_3^{(k)} \\ \Delta u_4^{(k)} \\ \Delta u_5^{(k)} \\ \Delta u_6^{(k)} \end{bmatrix} =$$

$$- \begin{bmatrix} u_1 - u_2 \\ u_1 - [2 + 0.12\, u_2^2]\, u_2 + u_3 + 0.00032 \\ u_2 - [2 + 0.12\, u_3^2]\, u_3 + u_4 + 0.00256 \\ u_3 - [2 + 0.12\, u_4^2]\, u_4 + u_5 + 0.00864 \\ u_4 - [2 + 0.12\, u_5^2]\, u_5 + u_6 + 0.02048 \\ u_6 - u_5 - 0.2 \end{bmatrix}$$

Note that Matrix is
- Tridiagonal
- Diagonally dominant
- Function of u_i's since ODE is non-linear

To solve the above problem,

- Guess $u_i^{(k)}$ for i = 1, 2, …6.
- Calculate **J** and ***f*** using $u_i^{(k)}$ for i = 1, 2, …6.
- Solve for $\Delta\mathbf{u}^{(k)}$ from $\quad \mathbf{J}\, \Delta\mathbf{u}^{(k)} = -\boldsymbol{f}$
- Check whether $\|\Delta\mathbf{u}^{(k)}\| <$ tol, or $\|\boldsymbol{f}\| <$ tol,

  where tol = 1×10^{-10} (desired accuracy)
  - If satisfied, $u_i^{(k)}$ is the solution.
  - If not satisfied, then
    - Calculate next estimate for u_i as $u_i^{(k+1)} = u_i^{(k)} + \Delta u_i^{(k)}$ for i = 1, 2, …6.

- Go to ____

Note that

- Matrix **J** is a tri-diagonal matrix independent of n with bandwidth of 3. Hence, one should use banded Gauss elimination (or banded **LU** decomposition) in solving **J** $\Delta\mathbf{u}^{(k)} = -\mathbf{f}$ problem in the course of Newton-Raphson iteration scheme since number of operations required by tri-diagonal matrix is 8n instead of n^3 operations (if we use full matrix GE or **LU** decomposition), where n is the size of the **J** matrix (which is equal to the number of unknowns, or nodes, or grids).
- Matrix **J** is diagonally dominant. Therefore, one can also use iterative methods (Jacobi or Gauss-Seidel method). Iterative method could be advantageous since it will guarantee convergence irrespective of initial guess values. Note that Newton-Raphson method may diverge for certain initial guess values but when it converge it converges quadratically. Whereas, iterative method will result in guaranteed convergence irrespective of starting initial guess values for the unknowns. However, the convergence rate will be linear. Therefore, decision is between robustness and convergence rate. Accuracy is not in question as it is dictated by the choice of number of grids and tolerance for convergence.
- Accuracy versus speed of computation: If we double the number of grid points, (which implies h $\rightarrow$ h/2), accuracy will increase (which means error will decrease) by a factor of 4 while computation (CPU) time will increase only by a factor of 2.

(v) When we increase the number of grids to 200 from 100, it means step size (distance between successive grids) will be reduced by a factor of 2. Since we are using central difference approximations for the derivatives, and we know that error for central difference approximation for derivatives is proportional to h^2, the accuracy will increase by a factor of 4 [$\equiv (½)^2$].

(vi) If we observe divergence for a particular set of initial guess value for the unknowns while using Newton-Raphson iterative scheme in solving a system of non-linear equations we can conclude that either (a) initial guess values were such that **J** matrix became singular or nearly singular (ill-conditioned), or, (b) there exist no solution.

3. Consider the following diffusion with irreversible chemical reaction in an isothermal porous catalyst slab described by

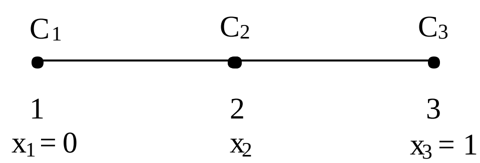
$$\frac{d^2C}{dx^2} - 2C^3 = 0$$

Boundary conditions: $C(x=0) = 1$

$$\left[\frac{dC}{dx} + C^2\right]_{x=1} = 0$$

where C and x are dimensionless concentration and position respectively.

We are interested in finding the numerical solution of the above problem by finite difference method using a total of only 3 nodes (1 interior node plus 2 boundary nodes). The variable naming scheme for the 3 nodes (or grids) is as follows:



Use central finite difference approximation for the interior node and forward or backward finite difference approximation for the boundary nodes.

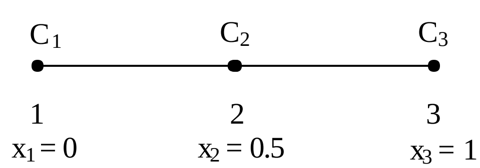
(a) Obtain the algebraic equations using the finite difference technique.

(b) Formulate the linear system of equations $\mathbf{J}^{(k)}\,\Delta\mathbf{C}^{(k)} = -\mathbf{f}^{(k)}$ you want to solve in the course of Newton-Raphson iteration.

(c) Determine the values of C_2 and C_3 after first iteration (i.e., $C_2^{(1)}$ and $C_3^{(1)}$) when initial guess values used are $C_2^{(o)} = 0.5$ and $C_3^{(o)} = 0$.

(d) Is the matrix, $\mathbf{J}^{(o)}$, in part (c) diagonally dominant? Can we use iterative method in the course of Newton-Raphson iteration?

<u>Solution</u>: $C'' - 2C^3 = 0$, $C(0) = 1$, $[C'(1) + C^2(1)] = 0$



(a)

$C_1 = 1$ ⇐ Boundary condition at grid # 1

$$\left[\frac{C_3 - 2C_2 + C_1}{h^2}\right] - 2C_2^3 = 0$$ ⇐ at interior grid # 2

$$\left[\frac{C_3 - C_2}{h}\right] + C_3^2 = 0$$ ⇐ Boundary condition at grid # 3

Simplifying 2nd equation, we have

$C_3 - 2\,C_2 + C_1 - 2\,h^2\,C_2^3 = 0$

or, $C_3 - 2\,[1 + h^2\,C_2^2]\,C_2 + C_1 = 0$

or, $C_3 - 2\,[1 + (0.5)^2\,C_2^2]\,C_2 = -1$ ⇐ Substituting $h = 0.5$, $C_1 = 1$

or, $-2\,[1 + 0.25\,C_2^2]\,C_2 + C_3 = -1$

Simplifying 3rd equation, we have

$C_3 - C_2 + h\,C_3^2 = 0$

or, $-C_2 + [1 + h\,C_3]\,C_3 = 0$

or, $-C_2 + [1 + 0.5\,C_3]\,C_3 = 0$

Therefore, the 2 non-linear equations for the 2 unknowns are as follow

$f_1(C_2, C_3) = 1 - 2\,[1 + 0.25\,C_2^2]\,C_2 + C_3 = 0$

$f_2(C_2, C_3) = -C_2 + [1 + 0.5\,C_3]\,C_3 = 0$

(b) To solve for C_2 and C_3, solve **J ΔC = -f**

i.e.,
$$\begin{bmatrix} \frac{\partial f_1}{\partial C_2} & \frac{\partial f_1}{\partial C_3} \\ \frac{\partial f_2}{\partial C_2} & \frac{\partial f_2}{\partial C_3} \end{bmatrix} \begin{bmatrix} C_2^{(k+1)} - C_2^{(k)} \\ C_3^{(k+1)} - C_3^{(k)} \end{bmatrix} = -\begin{bmatrix} f_1 \\ f_2 \end{bmatrix}$$

or,
$$\begin{bmatrix} -\left[2 + 1.5C_2^2\right] & 1 \\ -1 & 1 + C_3 \end{bmatrix} \begin{bmatrix} \Delta C_2 \\ \Delta C_3 \end{bmatrix} = -\begin{bmatrix} 1 - 2\left[1 + 0.25C_2^2\right]C_2 + C_3 \\ -C_2 + \left[1 + 0.5C_3\right]C_3 \end{bmatrix}$$

(c) If $C_2^{(0)} = 0.5$ and $C_3^{(0)} = 0$

Then we have

$$\begin{bmatrix} -2.375 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} \Delta C_2 \\ \Delta C_3 \end{bmatrix} = -\begin{bmatrix} -0.0625 \\ -0.5 \end{bmatrix}$$

or, $\begin{bmatrix}\Delta C_2\\ \Delta C_3\end{bmatrix} = -\dfrac{1}{-1.375}\begin{bmatrix}1 & -1\\ 1 & -2.375\end{bmatrix}\begin{bmatrix}0.0625\\ 0.5\end{bmatrix} = \begin{bmatrix}0.31818\\ 0.81818\end{bmatrix}$

Therefore, $\begin{bmatrix}C_2^{(1)}\\ C_3^{(1)}\end{bmatrix} = \begin{bmatrix}C_2^{(0)}\\ C_3^{(0)}\end{bmatrix} + \begin{bmatrix}\Delta C_2\\ \Delta C_2\end{bmatrix} = \begin{bmatrix}0.5\\ 0\end{bmatrix} + \begin{bmatrix}0.31818\\ 0.81818\end{bmatrix} = \begin{bmatrix}0.81818\\ 0.81818\end{bmatrix}$

(d) The matrix $\mathbf{J}^{(0)}$ is diagonally dominant and therefore, iterative method could also be used.

4. Consider the reaction plus diffusion problem

$$\frac{d^2C_A}{dx^2} = \left[\frac{k_1L_o^2}{D}\right]C_A = \alpha\ C_A$$

$$C_A(x=0)=1 \quad and \quad \frac{dC_A}{dx}(x=1)=0$$

where

$C_A = C_A/C_{Ao}$ = dimensionless concentration

C_{Ao} = concentration of A outside the reaction zone

$x = L/L_o$ = dimensionless position

L_o = thickness of the reaction zone

k_1 = rate constant for the reaction $A \rightarrow B$.

D = diffusion coefficient of A.

(a) Formulate and discuss two different methods for finding the concentration profile, C_A (x). Take α = 1.2

(b) If the original differential equation contains a non-linear rate expression of the form

$$\frac{d^2C_A}{dx^2} = \left[\frac{k_1L_o^2}{D}\right]\frac{C_A}{1+KC_A} = \frac{\alpha\ C_A}{1+KC_A}$$

How you are going to find out the concentration profile, C_A (x)?

Take K = 2.

<u>Solution:</u>

(a) $C'' - \alpha\, C = 0,\qquad C(0) = 1,\ C'(1) = 0$

Let $C' = S \qquad C(0) = 1$

Then $S' = \alpha\, C \qquad S(1) = 0$

To solve using the shooting method, guess a value for S(0), solve using Euler or 4th order RK method and check whether the value of S at x = 1 is 0. Since, the differential equation is linear one can find the exact guess value for S(0) after 2 trials.

Guess S(0)	Calculated S(1)
0.1	1.3295
-0.1	1.0209

Correct guess for S(0) can be obtained from

$S(0) = 0.1 + [(-0.1 - 0.1) / (1.0209 - 1.3295)]\ [0 - 1.3295] = -\ 0.7616$

Therefore, if we solve the following IVP

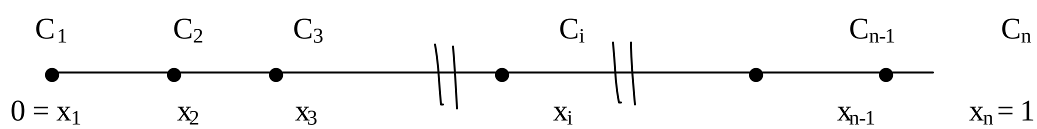
$C' = S \qquad C(0) = 1$

$S' = \alpha\, C \qquad S(0) = -0.7616$

using Euler or 4th order RK method (of course using proper h), it will satisfy the BVP

$C'' - \alpha\, C = 0,\qquad C(0) = 1,\ C'(1) = 0$

<u>Finite Difference method</u>: $C'' - \alpha\, C = 0,\qquad C(0) = 1,\ C'(1) = 0$



$C_1 = 1 \qquad \Leftarrow$ grid # 1 (Left boundary)

$$\left[\frac{C_{i-1} - 2C_i + C_{i+1}}{h^2}\right] - a\;\; C_i = 0, \qquad i = 2, 3, \ldots, n-1 \qquad \Leftarrow \text{grid \# i (interior grid \# i)}$$

or, $C_{i-1} - [2 + \alpha\, h^2]\, C_i + C_{i+1} = 0,\qquad i = 2, 3, \ldots, n-1$

$C'_n = 0 \qquad \Leftarrow$ grid # n (Right boundary)

or, $[C_n - C_{n-1}]\,/h = 0,\qquad$ or, $C_{n-1} = C_n$

- If we use iterative (for example, Gauss-Seidel) method to solve C_i's, then we have

  $C_1 = 1$

  $$C_i^{new} = \left[\frac{1}{2+\alpha h^2}\right]\left[C_{i-1}^{new} + C_{i+1}^{old}\right], \quad i = 2, 3, \ldots, n-1$$

  $C_n = C_{n-1}$

Note that the system is diagonally dominant

- If we use Newton-Raphson's method, then we have to solve

$$\mathbf{J}\,\Delta\mathbf{C} = -\boldsymbol{f}$$

For grid # 2, i = 2: $C_1 - [2 + \alpha h^2]\, C_2 + C_3 = 0$

or, $f_2 = 1 - [2 + \alpha h^2]\, C_2 + C_3 = 0$ $\Leftarrow$ since $C_1 = 1$

For grid # 3, i = 3: $C_2 - [2 + \alpha h^2]\, C_3 + C_4 = 0$

or, $f_3 = C_2 - [2 + \alpha h^2]\, C_3 + C_4 = 0$

For grid # 4, i = 4: $C_3 - [2 + \alpha h^2]\, C_4 + C_5 = 0$

or, $f_4 = C_3 - [2 + \alpha h^2]\, C_4 + C_5 = 0$

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For grid # n-2, i = n-2: $C_{n-3} - [2 + \alpha h^2]\, C_{n-2} + C_{n-1} = 0$

or, $f_{n-2} = C_{n-3} - [2 + \alpha h^2]\, C_{n-2} + C_{n-1} = 0$

For grid # n-1, i = n-1: $C_{n-2} - [2 + \alpha h^2]\, C_{n-1} + C_n = 0$

or, $C_{n-2} - [2 + \alpha h^2]\, C_{n-1} + C_{n-1} = 0$ $\Leftarrow$ since $C_n = C_{n-1}$

or, $C_{n-2} - [1 + \alpha h^2]\, C_{n-1} = 0$

or, $f_{n-1} = C_{n-2} - [1 + \alpha h^2]\, C_{n-1} = 0$

Therefore, we have to solve

$$\begin{bmatrix} -(2+\alpha h^2) & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -(2+\alpha h^2) & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -(2+\alpha h^2) & 1 & 0 & 0 & 0 \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ 0 & 0 & 0 & 1 & -(2+\alpha h^2) & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -(2+\alpha h^2) & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -(1+\alpha h^2) \end{bmatrix}$$

Note that

- Matrix is tri-diagonal
- Independent of C_i's

$$\times \begin{bmatrix} \Delta C_2 \\ \Delta C_3 \\ \Delta C_4 \\ \bullet \\ \bullet \\ \Delta C_{n-2} \\ \Delta C_{n-1} \end{bmatrix} = - \begin{bmatrix} f_2 \\ f_3 \\ f_4 \\ \bullet \\ \bullet \\ f_{n-2} \\ f_{n-1} \end{bmatrix}$$

To solve the above problem,

- Set $\alpha = 1.2$ (given), Choose n, then h = [1 - 0]/(n-1)
- Guess $C_i^{(0)}$ for i = 2, 3, …n-1.
- Calculate **J** and ***f*** using $C_i^{(0)}$ for i = 2, 3…n-1.
- Solve for $\Delta \mathbf{C}^{(0)}$ from $\mathbf{J}\, \Delta \mathbf{C}^{(0)} = -\boldsymbol{f}$
- Calculate $C_i^{(1)} = C_i^{(0)} + \Delta C_i^{(0)}$ for i = 2, 3…n-1.
- Since BVP is linear, $C_i^{(1)}$, for i = 2, 3…n-1, is the solution.

(b) $$C'' - \left[\frac{a}{1+KC}\right] C = 0\,, \qquad C(0) = 1,\; C'(1) = 0$$

Let $C' = S$ $\qquad C(0) = 1$

Then $S' = \left[\frac{a}{1+KC}\right] C$ $\qquad S(1) = 0$

To solve using the shooting method, guess a value for S(0), solve using Euler or 4th order RK method and check whether the value of S at x = 1 is 0. Since, the differential equation is non-linear, one can not find the exact guess value for S(0) after 2 trials.

Guess S(0)	Calculated S(1)
-1.2	-0.9494
-0.90	-0.5800
-0.70	-0.3512
-0.50	-0.1294
-0.40	-0.0203
-0.39	-0.0094
-0.38	-0.00145

Therefore, if we solve the following IVP

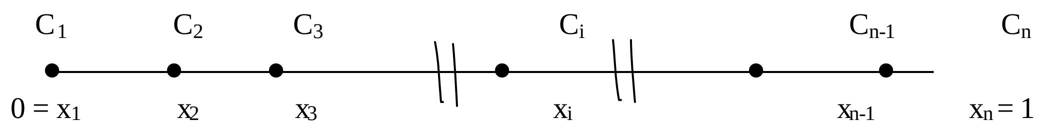
$$C' = S \qquad\qquad C(0) = 1$$

$$S' = \left[\frac{a}{1+KC}\right]C \qquad\qquad S(0) = -0.38$$

using Euler or 4th order RK method (of course using proper h), it will satisfy the BVP

$$C'' - \left[\frac{a}{1+KC}\right]C = 0, \qquad C(0) = 1,\ C'(1) = 0$$

<u>Finite Difference method</u>: $\quad C'' - \left[\frac{a}{1+KC}\right]C = 0, \qquad C(0) = 1,\ C'(1) = 0$



$C_1 = 1$ $\qquad\qquad \Leftarrow$ grid # 1 (Left boundary)

$$\left[\frac{C_{i-1} - 2C_i + C_{i+1}}{h^2}\right] - \left[\frac{a}{1+KC_i}\right] C_i = 0, \qquad i = 2, 3, \ldots, n-1 \qquad \Leftarrow \text{grid \# i (interior grid \# i)}$$

or, $\quad C_{i-1} - \left[2 + \frac{ah^2}{1+KC_i}\right]C_i + C_{i+1} = 0, \qquad i = 2, 3, \ldots, n-1$

$C'_n = 0$ $\qquad\qquad \Leftarrow$ grid # n (Right boundary)

or, $\quad [C_n - C_{n-1}]/h = 0$

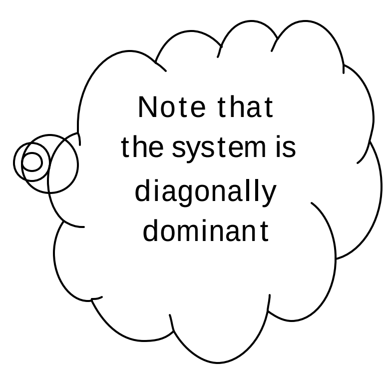
or, $\quad C_{n-1} = C_n$

If we use iterative (for example, Gauss-Seidel) method to solve C_i's, then we have

$C_1 = 1$

$$C_i^{new} = \left[\frac{1}{2 + \frac{a\,h^2}{1+KC_i^{old}}}\right]\left[C_{i-1}^{new} + C_{i+1}^{old}\right], \quad i = 2, 3, \ldots, (n-1)$$

$C_n = C_{n-1}$



If we use Newton-Raphson's method, then we have to solve

$$\mathbf{J}\,\Delta\mathbf{C} = -\boldsymbol{f}$$

For grid # 2, i = 2: $C_1 - \left[2 + \frac{a\,h^2}{1+KC_2}\right] C_2 + C_3 = 0$

or, $f_2 = 1 - \left[2 + \frac{a\,h^2}{1+KC_2}\right] C_2 + C_3 = 0$ $\Leftarrow$ since $C_1 = 1$

For grid # 3, i = 3: $C_2 - \left[2 + \frac{a\,h^2}{1+KC_3}\right] C_3 + C_4 = 0$

or, $f_3 = C_2 - \left[2 + \frac{a\,h^2}{1+KC_3}\right] C_3 + C_4 = 0$

For grid # 4, i = 4: $C_3 - \left[2 + \frac{a\,h^2}{1+KC_4}\right] C_4 + C_5 = 0$

or, $f_4 = C_3 - \left[2 + \frac{a\,h^2}{1+KC_4}\right] C_4 + C_5 = 0$

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For grid # n-2, i = n-2: $C_{n-3} - \left[2 + \frac{a\,h^2}{1+KC_{n-2}}\right] C_{n-2} + C_{n-1} = 0$

or, $f_{n-2} = C_{n-3} - \left[2 + \frac{a\,h^2}{1+KC_{n-2}}\right] C_{n-2} + C_{n-1} = 0$

For grid # n-1, i = n-1: $C_{n-2} - \left[2 + \frac{a\,h^2}{1+KC_{n-1}}\right] C_{n-1} + C_n = 0$

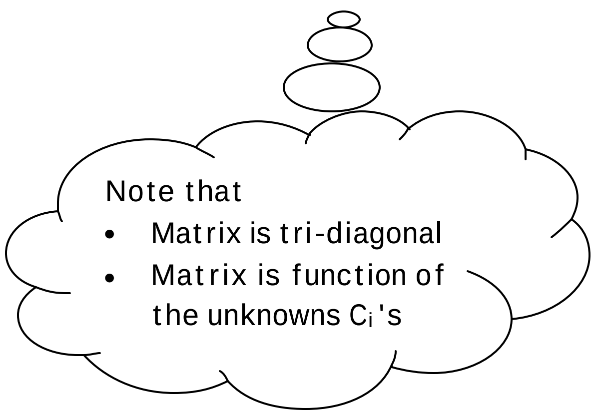
or, $C_{n-2} - \left[2 + \frac{a\,h^2}{1+KC_{n-1}}\right] C_{n-1} + C_{n-1} = 0$ $\Leftarrow$ since $C_n = C_{n-1}$

or, $C_{n-2} - \left[1 + \frac{a\,h^2}{1+KC_{n-1}}\right] C_{n-1} = 0$

or, $f_{n-1} = C_{n-2} - \left[1 + \frac{a\,h^2}{1+KC_{n-1}}\right] C_{n-1} = 0$

Therefore, in the course of Newton-Raphson's method, we have to solve the following

$$
\begin{bmatrix}
-\left[2+\frac{a\,h^2}{(1+KC_2)^2}\right] & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & -\left[2+\frac{a\,h^2}{(1+KC_3)^2}\right] & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & -\left[2+\frac{a\,h^2}{(1+KC_3)^2}\right] & 1 & 0 & 0 & 0 \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
0 & 0 & 0 & 0 & 1 & -\left[2+\frac{a\,h^2}{(1+KC_{n-2})^2}\right] & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & -\left[1+\frac{a\,h^2}{(1+KC_{n-1})^2}\right]
\end{bmatrix}
\times
\begin{bmatrix} \Delta C_2 \\ \Delta C_3 \\ \Delta C_4 \\ \bullet \\ \bullet \\ \Delta C_{n-2} \\ \Delta C_{n-1} \end{bmatrix}
= -
\begin{bmatrix} f_2 \\ f_3 \\ f_4 \\ \bullet \\ \bullet \\ f_{n-2} \\ f_{n-1} \end{bmatrix}
$$



To solve the above problem,

- Set α = 1.2 (given), K = 2 (given). Choose n, then h = [1 - 0]/(n-1)
- Guess $C_i^{(k)}$ for i = 2, 3, …n-1.
- Calculate **J** and ***f*** using $C_i^{(k)}$ for i = 2, 3…n-1.
- Solve for $\Delta \mathbf{C}^{(k)}$ from $\mathbf{J}\,\Delta \mathbf{C}^{(k)} = -\boldsymbol{f}$
- Check whether $||\Delta \mathbf{C}^{(k)}|| <$ tol, or $||\boldsymbol{f}|| <$ tol,
  where tol = 1×10^{-10} (desired accuracy)
  - If satisfied, $C_i^{(k)}$ is the solution.
  - If not satisfied, then
    - Calculate next estimate for C_i as $C_i^{(k+1)} = C_i^{(k)} + \Delta C_i^{(k)}$ for i = 2, 3,…(n-1).
    - Go to (step "Calculate **J** and ***f***")

5. Alternate mathematical models for steady-state heat conduction in a bar insulated at one end, which is uniformly heated throughout its length, are Model A and Model B below:

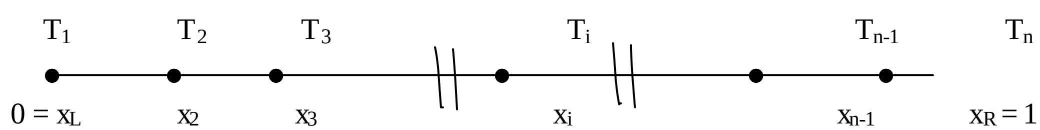
Model A:

$$\frac{d^2T}{dx^2} + a = 0, \quad T(x_L) = T_L, \quad \left.\frac{dT}{dx}\right|_{x_R} = 0$$

Model B:

$$\frac{d^2T}{dx^2} + b\left(T^{1/4} - g\right) = 0, \quad T(x_L) = T_L, \quad \left.\frac{dT}{dx}\right|_{x_R} = 0$$

The questions below pertain to attempted numerical solutions using central finite difference approximation of the equation using the variable naming scheme for the n total nodes shown below and use of Newton-Raphson iteration scheme to solve for the nodal variables T. The parameters α, β, γ, T_L, and T_R have fixed values.



(a) State the equation that applies for Model A at general interior node i.

(b) State the equation that applies for Model B at general interior node i.

(c) State the equation that applies for Model B at node n.

(d) Before you attempt to compute a solution for Model A, what are the possible significant outputs for any particular initial guess $\mathbf{T}^{(o)}$?

(e) Suppose your program converges to a solution for Model A for a particular initial guess $\mathbf{T}^{(o)}$.

  (i) Can you say how many iteration(s) will be required?

  (ii) Should you try a different initial guess?

(f) What would be the most appropriate linear system solver to implement for Model A and Model B?

(g) Before you attempt to compute a solution for Model B, what are the possible significant outputs for any particular initial guess $\mathbf{T}^{(o)}$?

(h) Suppose your program converges to a solution for Model B for a particular initial guess $\mathbf{T}^{(o)}$.

(i) Can you say how many iteration(s) will be required?

(ii) Should you try a different initial guess?

(i) Suppose the true solution for Model A is known. What would be the approximate slope of a plot of log [$E_t(X_R)$] vs. log [n] based on computed solutions for several values of n, where n >> 1?

Solution:

(a) $$\left[\frac{T_{i-1}-2T_i+T_{i+1}}{h^2}\right]+a=0, \qquad i = 2, 3, \ldots, (n-1).$$

or, $$f_i = T_{i-1} - 2T_i + T_{i+1} + a\,h^2 = 0 \qquad i = 2, 3, \ldots, (n-1).$$

(b) $$\left[\frac{T_{i-1}-2T_i+T_{i+1}}{h^2}\right]+b\left[T_i^{\frac{1}{4}}-g\right]=0 \qquad i = 2, 3, \ldots, (n-1).$$

or, $$f_i = T_{i-1} - \left[2 - b\,h^2 T_i^{-\frac{3}{4}}\right]T_i + T_{i+1} - bg\,h^2 = 0, \qquad i = 2, 3, \ldots, (n-1).$$

(c) $T'(x_R) = 0 \Rightarrow \quad f_n = -T_{n-1} + T_n = 0$

(d) Either unique solution or no solution as the BVP is linear.

(e) One iteration as the BVP is linear. There is no need to try any other initial guess values as when we get a converged solution, the solution is the only (unique) solution possible, and if we observe divergence, then there is no solution for the linear BVP.

(f) Banded Gauss elimination or banded **LU** decomposition (since the bandwidth of **J** matrix is 3) or iterative method as the system is diagonally dominant.

(g) Possible outcome: (i) convergence to a solution, (ii) divergence due to wrong initial guess values (for which **J** is singular or nearly singular) or due to no solution exist for the non-linear BVP, (iii) maximum number of iterations exceeded in the program, (iv) possibilities of many solutions do exist since the non-linear BVP resulted in non-linear systems of equation.

(h) Since the system of equations are non-linear, one will not be able to tell how many iterations would be required as it depends on initial guess values. One should try other initial guess values irrespective of whether convergence or divergence was achieved. If convergence was achieved, then one should try to find if there exist other solutions, as many solutions are possible from non-linear systems of equations. If however, divergence was observed, then also one should try other guess values to find a solution (if it exist) as Newton-Raphson method may diverge for some initial guess values.

(i) $E_t(x_R) \propto h^2 = \left[\frac{L}{n-1}\right]^2 \approx n^{-2}$ for n >> 1.

Therefore, $\log E_t = -2 \log n$

Slope = -2.