Modelling & Simulation of Chemical Engineering Systems

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LECTURE #10

Numerical Solution of Boundary-Value Differential Equations

Shooting Method

- An initial-value technique
- Use successive approximation to solve for the missing initial conditions.
- It can utilize highly efficient initial value procedure.
- Shooting can be tried from either end of the BVP.

Shooting Method Algorithm

$$\frac{dy_1}{dx} = f_1(x, y_1, y_2) \qquad y_1(x_o) = y_{10}$$

$$\frac{dy_2}{dx} = f_1(x, y_1, y_2) \qquad y_2(x_f) = y_{2f}$$

- Problem:
- Guess initial condition for y_2 :

$$y_2(x_o) = \gamma$$

- Integrate the system forward, calculated y_2 at x_f is

$$y_2(x_f)\Big|_{calculated} = y_2(x_f, \gamma)$$

- Define the function

$$\phi(\gamma) = y_2(x_f, \gamma) - y_{2f} = 0$$

- Solution :

Nonlinear function need to be solved for γ

$$\Delta\gamma = \frac{-\phi(\gamma)}{\left[\frac{\partial\phi}{\partial\gamma}\right]} \qquad \gamma_{new} = \gamma_{old} + \rho\Delta\gamma, \qquad 0 < \rho \le 1$$

$$\frac{\partial \phi}{\partial \gamma} = \frac{\partial (y_2(x_f,\gamma) - y_{2f})}{\partial \gamma} = \frac{\partial y_2(x_f,\gamma)}{\partial \gamma}$$

Differntiate the original differential equations

$$\frac{\partial}{\partial \gamma}\left(\frac{dy_1}{dx}\right) = \frac{d}{dx}\left(\frac{\partial y_1}{\partial \gamma}\right) = \frac{\partial f_1}{\partial y_1}\frac{\partial y_1}{\partial \gamma} + \frac{\partial f_1}{\partial y_2}\frac{\partial y_2}{\partial \gamma}$$

$$\frac{\partial}{\partial \gamma}\left(\frac{dy_2}{dx}\right) = \frac{d}{dx}\left(\frac{\partial y_2}{\partial \gamma}\right) = \frac{\partial f_2}{\partial y_1}\frac{\partial y_1}{\partial \gamma} + \frac{\partial f_2}{\partial y_2}\frac{\partial y_2}{\partial \gamma}$$

Define the sensitivity functions

$$v_1 = \left(\frac{\partial y_1}{\partial \gamma}\right), \qquad v_2 = \left(\frac{\partial y_2}{\partial \gamma}\right)$$

$$\frac{dv_1}{dx} = \frac{\partial f_1}{\partial y_1} v_1 + \frac{\partial f_1}{\partial y_2} v_2 \qquad v_1(a) = \left(\frac{\partial y_1}{\partial \gamma}\right)_a = 0$$

$$\frac{dv_2}{dx} = \frac{\partial f_2}{\partial y_1} v_1 + \frac{\partial f_2}{\partial y_2} v_2 \qquad v_2(a) = \left(\frac{\partial y_2}{\partial \gamma}\right)_a = 1$$

HW

- Solve the problem of flow of a Newtonian flow fluid in a pipe described by the equation:
- Compare the solutions obtained using the shooting method, finite difference and MATLAB bvp4c solver

$$\frac{d^2v}{dr^2} = -\frac{1}{\mu}\frac{\Delta p}{L} - \frac{1}{r}\frac{dv}{dr}$$

$$\frac{dv}{dr}(r=0) = 0, \qquad v(r=R) = 0$$

$$R = 0.0025$$

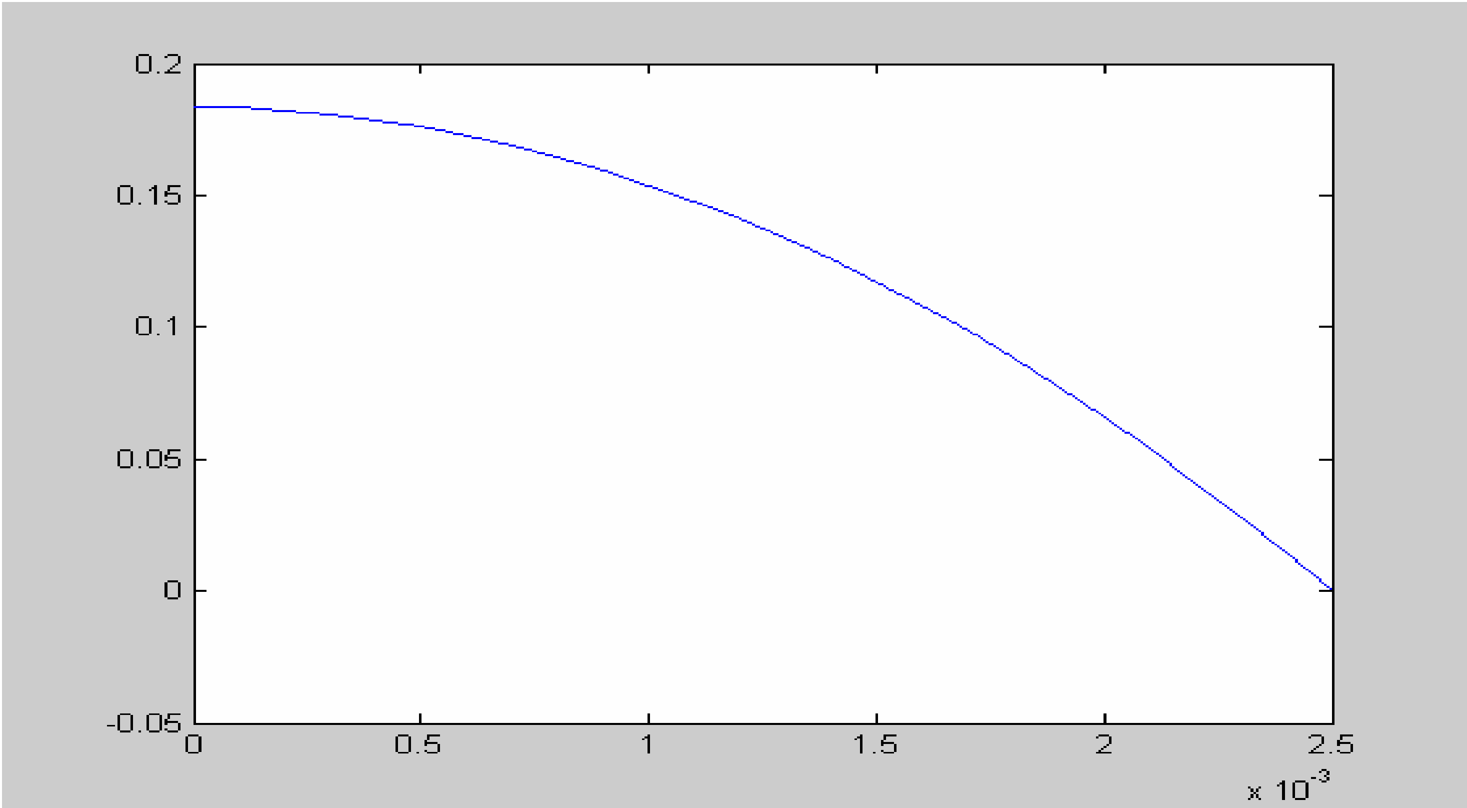
$$\Delta p = 2.8 \times 10^5$$

$$\mu = 0.492$$

$$L = 4.88$$

```
% Canonical Form : z1= y, z2=y', z3=v, z4=v'
% z1'= z2              =f1
% z2'= -1/mu*DP/L-1/rz2  =f2
% z3'= df1/dz1*z3+df1/dz2*z4 = z4
% z4'= df2/dz1*z3+df2/dz2*z4 =-1/r*z4
R=0.0025
yb=0
eps=0.0001;
maxiter=10;
a=0; b=R;
rspan=[a:0.0001:b];
i=1;
t(i)=0.3
tol=1.0
while ((tol > eps) & i< maxiter)
   z0=[t(i) 0 1 0]';
   [x,z]=ode23('funchw9', rspan, z0)
   [n,nn]=size(z)
   m(i)=z(n,1)-yb
   tol=abs(m(i));
   t(i+1)=t(i)-m(i)/z(n,3)
   i=i+1;
end
plot(x,z(:,1));
```

```
function zp=funchw9(x,z)
% z1'= z2              =f1
% z2'= -1/mu*DP/L-1/rz2  =f2
% z3'= df1/dz1*z3+df1/dz2*z4 = z4
% z4'= df2/dz1*z3+df2/dz2*z4 =-1/r*z4
mu=0.492; DP=2.8*10^5; L=4.88; R=0.0025;
par=-1/mu*DP/L
zp(1)=z(2);
zp(2)=par-1/(x+0.00001)*z(2);
zp(3)=z(4);
zp(4)=-1/(x+0.00001)*z(4);
zp=zp'
```


0.2
0.15
0.1
0.05
0
-0.05
0
0.5
1
1.5
2
2.5
x 10^-3

Finite Difference Method

$$\frac{d^2v}{dr^2} = \text{-1.1662e+005} - \frac{1}{r}\frac{dv}{dr} \qquad \frac{dv}{dr}(r=0)=0, \quad v(r=R)=0$$

$$r\frac{d^2v}{dr^2} = r * \text{-1.1662e+005} - \frac{dv}{dr}$$

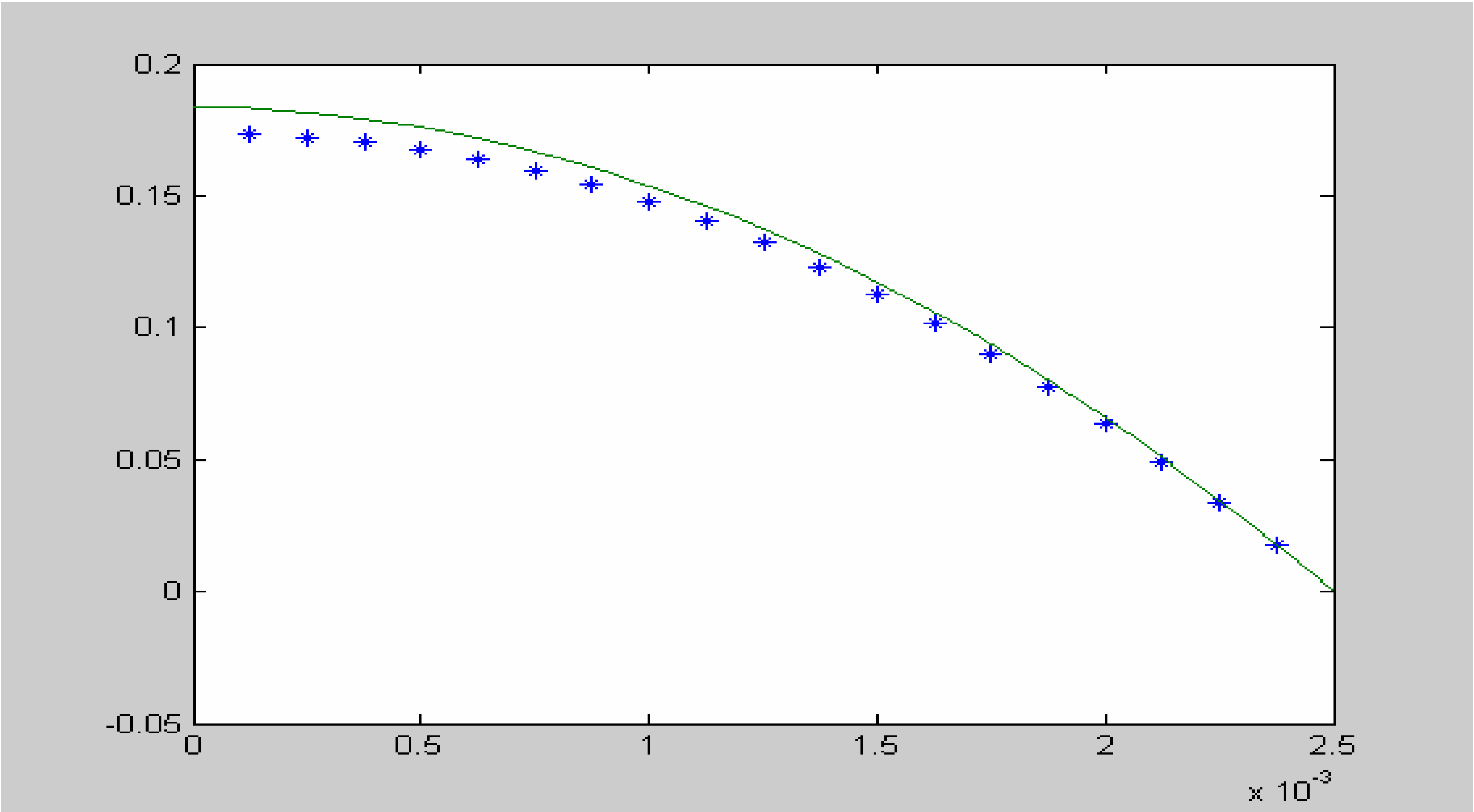
$$(ih)\frac{v_{i+1}-2v_i+v_{i-1}}{h^2} = ih \times (\text{-1.1662e+005})\text{-}\frac{v_{i+1}-v_i}{h}$$

$$i = 1\ldots,(R-h)/h$$

```
R=0.0025
N=20
h=R/20
for n=1:N-1
    r(n)=n*h
    vo(n)=0.1
end
v=fsolve('bvp_fd1',vo)
```

```
function f=bvp_fd1(v)
%f= i*h*(v(i+1)-2v(i)+v(i-1))/h^2+1.166*10^5*i*h+(v(i+1)-v(i))/h
% Span; 0: R
% h=R/10
R=0.0025
N=20 % number of nodes
h=R/N;
% First Boundary condition
v0=v(1)
%First node
i=1
f(1)=i*h*(v(i+1)-2*v(i)+v0)/h^2+1.166*10^5*i*h+(v(i+1)-v0)/h;

for i=2:N-2
  f(i)=i*h*(v(i+1)-2*v(i)+v(i-1))/h^2+1.166*10^5*i*h+(v(i+1)-v(i))/h;
end
%Last node
v(N)=0
i=N-1
f(i)=i*h*(0-2*v(i)+v(i-1))/h^2+1.166*10^5*i*h+(0-v(i))/h;
```


0.2
0.15
0.1
0.05
0
-0.05
0
0.5
1
1.5
2
2.5
x 10-3

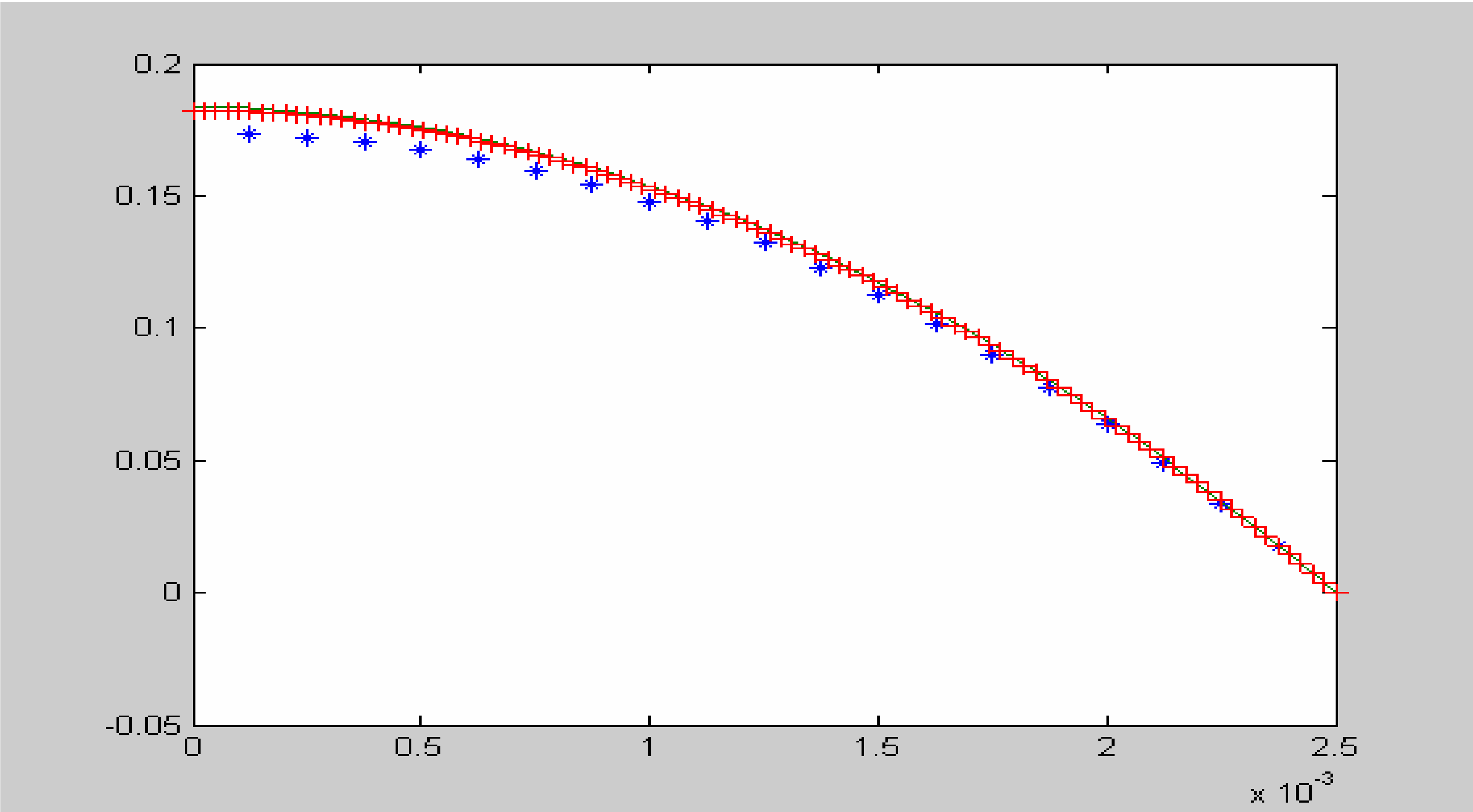
MATLAB command

```
function dydr = ge501pvb2(r,y)
% y''=-1/mu*DP/L-1/ry' y'(0)=0, y(R)=0
mu=0.492; DP=2.8*10^5; L=4.88; R=0.0025;
par=-1/mu*DP/L
dydr = [ y(2);  par-1/(r+0.000000001)*y(2)];
```

```
function res = ge501_bc2(ya,yb)
res = [ ya(2);   yb(1) ];
```

```
solin=bvpinit([0 0.001 0.0015 0.002 0.0025],[0.1 0.1]);

 sol=bvp4c(@ge501pvb2,@ge501_bc2,solin);
 rint=linspace(0,0.0025);
 vint=deval(sol,rint);
 plot(rint,vint(1,:))
```



0.2
0.15
0.1
0.05
0
-0.05
0
0.5
1
1.5
2
2.5
x 10-3

Methods of Weighted Residuals

- Reduces domain dimensions
- Approximates solution by ”trial” function
- Trial function form is specified but has adjustable coefs.
- Trial function chosen so as to satisfy BCs
- For efficiency → trial functions are linearly independent!
- Residual (distance between exact and approximated
- solns.) made zero

MWR Concept

Linear Differential operator

$$D(u(x)) = p(x) \qquad (1)$$

approximate u by $\bar{u}$

$$u \cong \bar{u} = \sum_{i=1}^{n} a_i \varphi_i \qquad (2)$$

substitution into eq.1

$$R(x) = D(\bar{u}(x)) - p(x) \neq 0 \qquad \text{Residual}$$

MWR objective

$$\int_X R(x) W_i(x) dx = 0 \qquad i = 1, 2, ..n$$

Number of weight functions W = Number of unknown constants a_i in $\bar{u}$

MWR objective

$$\int_X R(x)W_i(x)dx = 0 \qquad i = 1,2,..n$$

MWR methods

1. Collocation method

$$\mathrm{W_i}(x) = \delta(x - x_i) \Rightarrow \int_X R(x)W_i(x)dx = R(x_i) = 0$$

2. Subdomain method

$$\int_X R(x)W_i(x)dx = \sum_i \int_{X_i} R(x_i)dx = 0$$

3. Least Square method $\mathrm{W_i}(x) = \dfrac{\partial R}{\partial a_i}$

4. Galerkin method $\mathrm{W_i}(x) = \dfrac{\partial \overline{u}}{\partial a_i}$

5. Method of moments $\mathrm{W_i}(x) = x^i$

Example

$$\frac{d^2v}{dr^2} = \text{-1.1662e+005} - \frac{1}{r}\frac{dv}{dr} \qquad \frac{dv}{dr}(r=0)=0, \qquad v(r=R)=0$$

Approximate solution

$$\bar{v} = a_o + a_1 r + a_2 r^2$$

application of Boundary conditions

$$\bar{v}(r=R) = 0 = a_o + a_1 R + a_2 R^2$$

$$\frac{dv}{dr}(r=0) = 0 = a_1$$

$$a_1 = 0, \qquad a_o = -a_2 R^2$$

$$\bar{v} = a_2(r^2 - R^2)$$

$$\frac{d\bar{v}}{dr} = 2a_2 r \qquad \frac{d^2\bar{v}}{dr^2} = 2a_2$$

Residual

$$\text{R(r)} = \frac{d^2v}{dr^2} + \text{1.1662e+005} + \frac{1}{r}\frac{dv}{dr}$$

$$= 2a_2 + \text{1.1662e+005} + \frac{1}{r}2a_2 r = 0$$

$$a_2 = -\text{1.1662e+005}/4$$

As an example, consider the solution of the following mathematical problem. Find $u(x)$ that satisfies

$$\begin{aligned} \frac{d^2u}{dx^2} + u &= 1 \\ u(0) &= 1 \end{aligned}$$

Let's solve by the Method of Weighted Residuals using a polynomial function as a basis. That is, let the approximating function $\widetilde{u}(x)$ be

$$\widetilde{u}(x) = a_0 + a_1 x + a_2 x^2.$$

Application of the boundary conditions reveals

$$\begin{aligned} \widetilde{u}(0) &= 1 = a_0 \\ \widetilde{u}(1) &= 0 = 1 + a_1 + a_2 \end{aligned}$$

or

$$a_1 = -(1 + a_2)$$

and the approximating polynomial which also satisfies the boundary conditions is then

$$\begin{aligned} \widetilde{u}(x) &= 1 - (1 + a_2)x + a_2 x^2 \\ &= 1 - x + a_2(x^2 - x). \end{aligned}$$

To find the residual $R(x)$, we need the second derivative of this function, which is simply $d^2\widetilde{u}/dx^2 = 2a_2$. So the residual is

$$\begin{aligned} R(x) &= \frac{d^2\widetilde{u}}{dx^2} + \widetilde{u} - 1 \\ &= 2a_2 + (1 - x + a_2(x^2 - x)) - 1 \\ &= -x + a_2(x^2 - x + 2) \end{aligned}$$

2.6.1 Collocation Method

For the collocation method, the residual is forced to zero at a number of discrete points. Since there is only one unknown (a_2), only one collocation point is needed. We choose (arbitrarily, but from symmetry considerations) the collocation point $x = 0.5$. Thus, the equation needed to evaluate the unknown a_2 is

$$R(0.5) = -0.5 + a_2(0.25 - .5 + 2) = 0$$

So

$$a_2 = +0.5/1.75 = 2/7 = 0.285714$$

2.6.4 Galerkin Method

In the Galerkin Method, the weight function W_1 is the derivative of the approximating function $\tilde{u}(x)$ with respect to the unknown coefficient a_2:

$$W_1(x) = \frac{d\tilde{u}}{da_2} = x^2 - x$$

So the weighted residual statement becomes

$$\begin{aligned} \int_0^1 W_1(x) \cdot R(x) dx &= 0 \\ \int_0^1 \left(x^2 - x\right) \cdot \left[-x + a_2(x^2 - x + 2)\right] dx &= 0 \end{aligned}$$

Again, the math is straightforward but tedious. Direct evaluation leads to the algebraic equation:

$$\frac{1}{12} - \frac{3}{10}a_2 = 0$$

So

$$a_2 = \frac{1}{12} \cdot \frac{10}{3} = 5/18 = 0.27\overline{7}$$

Table 2.1: Comparison of Different Approximations in Example 1.

x	exact	collocation	Subdomain	LeastSquares	Galerkin
0.00	1.0000	1.0000	1.0000	1.0000	1.0000
0.05	0.94060	0.93643	0.93705	0.93707	0.93681
0.10	0.88136	0.87429	0.87545	0.87550	0.87500
0.15	0.82241	0.81357	0.81523	0.81528	0.81458
0.20	0.76390	0.75429	0.75636	0.75644	0.75556
0.25	0.70599	0.69643	0.69886	0.69895	0.69792
0.30	0.64881	0.64000	0.64273	0.64282	0.64167
0.35	0.59250	0.58500	0.58795	0.58806	0.58681
0.40	0.53722	0.53143	0.53455	0.53465	0.53333
0.45	0.48309	0.47929	0.48250	0.48261	0.48125
0.50	0.43025	0.42857	0.43182	0.43193	0.43056
0.55	0.37884	0.37929	0.38250	0.38261	0.38125
0.60	0.32898	0.33143	0.33455	0.33465	0.33333
0.65	0.28080	0.28500	0.28795	0.28806	0.28681
0.70	0.23441	0.24000	0.24273	0.24282	0.24167
0.75	0.18994	0.19643	0.19886	0.19895	0.19792
0.80	0.14750	0.15429	0.15636	0.15644	0.15556
0.85	0.10718	0.11357	0.11523	0.11528	0.11458
0.90	0.06910	0.07429	0.07545	0.07550	0.07500
0.95	0.03334	0.03643	0.03705	0.03707	0.03681
1.00	0.00000	0.00000	0.00000	0.00000	0.00000
	RMS Errors	0.00591	0.00584	0.00585	0.00576

HW.5

- Consider the reaction-diffusion problem in a spherical domain. The reaction rate expression is used to describe the Michaelis-Menten reaction in Biological systems. The nondimensional form is given as

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dc}{dr}\right)=\frac{\alpha c}{1+Kc}, \qquad \frac{dc(0)}{dr}=0 \quad c(1)=1$$

$$\alpha=5, K=2$$

- Solve the problem using:
  - Shooting method
  - Finite difference method
  - MATLAB bvp4c
  - MWR methods
  - FEMLAB