# Numerical analysis by 1D FEMLAB

# Root finding

$$f(u) = f(u_0) + (u - u_0)f'(u_0) + \cdots , \tag{1}$$

which can be re-arranged, ignoring higher order terms in $(u - u_0)$ to estimate the root as

$$u = u_0 - \frac{f(u_0)}{f'(u_0)} . \tag{2}$$

Start up MATLAB and type COMSOL Multiphysics in the command window. After several splash screens, you should be facing the Model Navigator window. Follow the steps in Table 1 to set up a 0-D application mode to solve the nonlinear polynomial equation:

$$u^3 + u^2 - 4u + 2 = 0 . \tag{3}$$

Physics: Subdomain settings specifies the equation to be satisfied in each subdomain in Table 1. Notice the equation in the upper left given in vector notation. In 1-D, this equation can be simplified to

$$d_a \frac{\partial u}{\partial t} - \frac{\partial}{\partial x}\left(c\frac{\partial u}{\partial x} + \alpha u\gamma\right) + au + \beta\frac{\partial u}{\partial x} = f . \tag{4}$$

Clearly, $\alpha\gamma$ and $\beta$ are redundant with the simplification to 1-D. Since we want to find roots in 0-D, however, all the coefficients on the LHS of (4) can be set to zero. By rearranging the polynomial, we can readily see that $a = 4$ and $f = u^3 + u^2 + 2$. Note that we discretize the domain with a single element by specifying the maximum element size to be one, giving us 0-D!

# FEMLAB

Table 1. Root finding example in coefficient mode. File name: rootfinder.mph.

| | |
|---|---|
| Model Navigator | Select 1-D. COMSOL Multiphysics:PDE modes:PDE, coefficient form |
| Draw Menu | Specify objects: Line. Coordinates pop-up menu. $x$ : 0 1 name: interval OK |
| Physics Menu: Boundary settings | Select domains: 1 and 2 (hold down Ctrl key)<br>Select Neumann boundary conditions<br>Leave defaults $q = 0$ $g = 0$ OK |
| Physics Menu: Subdomain settings | Select domain: 1<br>Set $c = 0$; $a = 4$; $f = u\hat{}3 + u\hat{}2 + 2$; $d_a = 0$<br>Apply. Select init tab: set $u(t_0) = -2$ OK |
| Mesh menu: mesh parameters | Set maximum element size 1<br>Hit remesh. OK |
| Solve menu: solver parameters | Stationary nonlinear. Solve. OK |
| Post-processing: Point Evaluation | Boundary selection: 1. Expression: $u$. OK |

By specifying the initial guess of as $u(t_0) = -2$, we find the root nearest to this value. If you are wondering why $a = 4$ was set, rather than all of the dependence put into $f$, it is so that the finite element discretization of the RHS of (4) does not result in a singular stiffness matrix.

The post-processing stage shows the result in the output window:

$$\text{Value} : -2.732051, \text{Expression} : u, \text{Boundary} : 1\,.$$

# General root finding

Table 2. Root finding example in general mode. File name: rtfindgen.mph.

| | |
|---|---|
| Model Navigator | 1-D, COMSOL Multiphysics:PDE modes, general form |
| Options | Set Axes/Grid to [0,1] |
| Draw | Name: Interval; Start = 0; Stop = 1 |
| Physics Menu/ Boundary Settings | Set both endpoints (domains) to Neumann BCs |
| Physics Menu/Subdomain Settings | set $\Gamma = 0$; $d_a = 0$; $F = u^3 + u^2 - 4 * u + 2$ |
| Mesh mode | Set Max element size, general = 1; Remesh |
| Solve | Use default settings (nonlinear solver, exact Jacobian) |
| Post-process | After five iterations, the solution is found. Click on the graph to read out $u = 0.732051$. Play with the initial conditions to find the other two roots |

Table 3. Root finding in ODE settings.

| | |
|---|---|
| Physics Menu: ODE settings | Name: $v$. Equation: $\tanh(v) - v^{\wedge}2 + 5$ OK |
| Solve menu: solver parameters | Stationary nonlinear. Solve. OK |
| Post-processing | Point evaluation. Boundary 2. Expression: $v$ |
| Report window | Value: $-2.008819$, Expression: $v$, Boundary: 2 |

# Root finding in flash distillation

A liquid hydrocarbon mixture undergoes a flash to 3.4 bar and 65°C. The composition of the liquid feed stream and the "$K$" value of each component for the flash condition are given in the table. We want to determine composition of the vapor and liquid product streams in a flash distillation process and the fraction of feed leaving the flash as liquid. Table 4 gives the initial composition of the batch.

Table 4. Initial composition to the flash unit and partition coefficients $K$ at equilibrium.

| Component | $X_I$ | $K_i$ at 65°C and 3.4 bar |
|---|---|---|
| Ethane | 0.0079 | 16.2 |
| Propane | 0.1281 | 5.2 |
| *i*-Butane | 0.0849 | 2.6 |
| *n*-Butane | 0.2690 | 1.98 |
| *i*-Pentane | 0.0589 | 0.91 |
| *n*-Pentane | 0.1361 | 0.72 |
| Hexane | 0.3151 | 0.28 |

A material balance for component $i$ gives the relation

$$X_i = (1-\phi)y_i + \phi x_i\,,$$

$$y_i = \frac{X_i}{1-\phi(1-\frac{1}{K_i})}\,.$$

$$f(\phi) = 1 - \sum_{i=1}^{n} \frac{X_i}{1-\phi(1-\frac{1}{K_i})} = 0\,,$$

where $X_i$ is the mole fraction in the feed (liquid), $x_i$ is the mole fraction in the liquid product stream, $y_i$ is the mole fraction in the vapour product, and $\phi$ is the ratio of liquid product to feed molar flow rate. The definition of the equilibrium coefficient is $K_i = y_i/x_i$. Using this to eliminate $x_i$ from the balance relation results in a single equation between $y_i$ and $X_i$:

# Root finding in flash distillation

Table 5. Flash distillation example.

| | |
|---|---|
| Model Navigator | Select 1-D. COMSOL Multiphysics:PDE modes:PDE, general form |
| Draw Menu | Specify objects: Line. Coordinates pop-up menu. $x$: 0 1 name: interval OK |
| Options: Constants | Enter the data from Table 4<br>$X_1$, 0.0079, etc. |
| Options: Scalar Expressions | Define expression for the terms in the RHS of (8)<br>$t_1 - X_1/(1 - u * (1 - 1/K_1))$<br>$t_2 - X_2/(1 - u * (1 - 1/K_2))$ etc. |
| Physics Menu: Boundary settings | Select domains: 1 and 2 (hold down Ctrl key)<br>Select Neumann boundary conditions<br>Leave defaults $q = 0$ $g = 0$ OK |
| Physics Menu: Sub-domain settings | Select domain: 1<br>Set $F = 1 + t_1 + t_2 + \cdots + t_7$; $d_a = 0$<br>Select Init tab; set $u(t_0) = 0.5$ |
| Mesh menu: mesh parameters | Set maximum element size 1<br>Hit remesh. OK |
| Solve menu: solver parameters | Stationary nonlinear. Solve. OK |
| Post-processing: Point Evaluation | Boundary selection: 1. Expression: $u$. OK<br>Report window: Value : 0.458509, Expression: $u$ |

# Numerical integration

$$\frac{d^2y}{dx^2} + q(x)\frac{dy}{dx} = r(x)$$

$$\frac{dy}{dx} = z(x)\,,$$
$$\frac{dz}{dx} = r(x) - q(x)z(x)\,.$$

$$\frac{d^2u}{dt^2} + u = 0$$

Reduction of order yields two first order ODEs:

$$\frac{du_1}{dt} = -u_2\,,$$
$$\frac{du_2}{dt} = u_1\,.$$

Table 6. Time integration by marching of a simple example.

| | |
|---|---|
| Model Navigator | Select 1-D. COMSOL Multiphysics:PDE modes:PDE, general form Insert dependant variables: $u_1 u_2$<br>Select Element: Lagrange-Linear |
| Draw Menu | Specify objects: Line. Coordinates pop-up menu. $x$: 0 1<br>name: interval OK |
| Physics Menu: Boundary settings | Select domains: 1 and 2 (hold down Ctrl key)<br>Select Neumann boundary conditions<br>Leave defaults $q = 0$ $g = 0$ OK |
| Physics Menu: Sub-domain settings | Select domain: 1<br>Set $F_1 = -u_2$, $F_2 = u_1$;<br>Select Init tab; set $u_1(t_w) = 1$ |
| Mesh menu: mesh parameters | Set maximum element size 1<br>Hit remesh. OK |
| Solve menu: solver parameters | Time-dependent solve. Enter on General tab<br>Times: linspace (0, 2*pi, 50)<br>Solve. OK |
| Post-processing: Cross-section plot parameters | Point tab. Accept the default of $u_1$<br>General tab. Accept the default of all times<br>OK |

# Reactor design by ODE's

A tubular reactor is used to dehydrate gaseous ethyl alcohol at 2 bar and 150°C. The formula for this chemical reaction is

$$C_2H_5OH \rightarrow C_2H_4 + H_2O\,.$$

Some experiments on this reaction have suggested the reaction rate expression at 2 bar pressure and 150°C, where $C_A$ is the concentration of ethyl alcohol (mol/litre) and $R$ is the rate of consumption of ethyl alcohol (mol/s/m$^3$):

$$R = \frac{52.7C_A^2}{1 + \frac{0.013}{C_A}}\,.$$

The reactor is to have a 0.05 m diameter and the alcohol inlet flowrate is to be 10 g/s. The objective is to determine the reactor length to achieve various degrees of alcohol conversion. We wish to determine reactor length for the outlet alcohol mole fractions 0.5, 0.4, 0.3, 0.2, and 0.1.

$$\frac{dC_A}{dt} = -R\left(1 + \frac{C_A}{C}\right),$$
$$\frac{dC_W}{dt} = R\left(1 - \frac{C_W}{C}\right),$$
$$\frac{dV}{dt} = \frac{RV}{C},$$
$$\frac{dx}{dt} = V.$$

$$C_A(0) = C \qquad V(0) = V_0,$$
$$C_W(0) = 0 \qquad x(0) = 0.$$

Assuming small heat of reaction, plug flow and ideal gas behaviour, it can be shown that the reacting flow is described by four ordinary differential equations in terms of the dependent variables $C_A$, $C_W$ (the water concentration), $V$ (the velocity) and $x$ (the distance along the reactor from the inlet):

Table 7. Tubular reactor design modelling steps in COMSOL Multiphysics.

| | |
|---|---|
| Model Navigator | Select 1-D. COMSOL Multiphysics:PDE modes:PDE, general form<br>Set dependent variables: $u_1 u_2 u_3 u_4$<br>Select Element: Lagrange-Linear. OK |
| Draw Menu | Specify objects: Line. Coordinates pop-up menu. $x$: 0 1<br>name: interval OK |
| Options Menu: Constants | Fill out the table as below<br>Name Expression<br>P 200000<br>T 423<br>R 8314<br>MM 46<br>Flowrate 0.01<br>Dia 0.05<br>C P/(RT)<br>area pi*Dia^2/4<br>rho MM*C<br>vel Flowrate/rho/area<br>OK |
| Options Menu: Scalar Expressions | Define rate = $52.7 * u_1\hat{}2/(1 + 0.013/u_1)$ |
| Physics Menu: Boundary settings | Select domains: 1 and 2 (hold down Ctrl key)<br>Select Neumann boundary conditions<br>Leave defaults $q = 0$ $g = 0$ OK |
| Physics Menu: Sub-domain settings | Select domain 1<br>$F$ tab; set $F_1 = -\text{rate} * (1 + u_1/C)$; $F_2 = \text{rate} * (1 - u_2/C)$; $F_3 = \text{rate} * u_3/C$; $F_4 = u_3/C$<br>Init tab; set $u_1(t_0) = C$; $u_3(t_0) =$ vel. OK |
| Mesh menu: mesh parameters | Set maximum element size 1<br>Hit remesh. OK |
| Solve menu: solver parameters | Time-dependent solve. Enter on General tab<br>Times: linspace (0, 10, 100)<br>Solve. OK |
| Post-processing: Cross-section plot parameters | Point tab. Accept the default of $u_1$<br>General tab. Accept the default of all times<br>OK |

# Reaction Diffusion Eqn

One of the major advantages of the finite element method is that it naturally solves two-point BVPs. As an example, the reaction and diffusion equation in 1-D is

$$\frac{D}{L^2}\frac{\partial^2 u}{\partial x^2} = R(u)\,,$$

where $u$ is the concentration of the species, $D$ is the diffusivity, $L$ is the length of the domain, $R(u)$ is the disappearance rate by reaction, and $x$ is the dimensionless spatial coordinate. If the unknown function $u(x)$ is approximated by discrete values $u_j = u(x_j)$ at the grid points $x = x_j = j\Delta x$, then with central differences, the system of equations becomes

$$\sum_{j=1}^{N} M_{ij} u_j = \frac{L^2 \overline{\Delta x}^2}{D} R_i\,,$$

where $M_{ij}$ is a tridiagonal matrix with the diagonal element $-2$, and 1 on the super and subdiagonals:

$$M = \begin{bmatrix} -2 & 1 & 0 & 0 & \cdots \\ 1 & -2 & 1 & 0 & \cdots \\ 0 & 1 & \ddots & \ddots & \ddots \\ 0 & 0 & \ddots & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix},$$

We will now illustrate the solution of (21) with COMSOL Multiphysics on a small 1-D domain with first order reaction $R(u) = ku$ and representative values for the resulting dimensionless parameter, the Damkohler number:

$$Da = \frac{kL^2}{D} = \frac{(10^{-3}\ \mathrm{s}^{-1})(10^{-3}\ \mathrm{m}^{-1})^2}{1.2 \times 10^{-9}\ \mathrm{m}^2/\mathrm{s}} = 0.833\,,$$

and with boundary conditions $u = 1$ at $x = 0$ and no flux at $u = 1$.

Table 8. ODE example of a two-point boundary value problem in a reaction-diffusion system.

| | |
|---|---|
| Model Navigator | Select 1-D. COMSOL Multiphysics:PDE modes:PDE, *coefficient* form<br>Set dependent variable: $u$<br>Select Element: Lagrange-Linear. OK |
| Draw Menu | Specify objects: Line. Coordinates pop-up menu. $x$: 0 1 name: interval OK |
| Physics Menu: Boundary settings | Select domains 1<br>Check Dirichlet and set $h = 1$; $r = 1$<br>Select domain 2<br>Select Neumann boundary conditions. OK |
| Physics Menu: Subdomain settings | Select domain 1<br>Set $C = -1$; $f = 0.833 * u$; $d_a = 0$<br>Select Init tab; set $u(t_0) = 1 - x$<br>OK |
| Meshing | Click on triangle symbol to mesh |
| Solve menu: solver parameters | Note stationary linear default. OK<br>General tab. Set solution form to "Coefficient"<br>Solve with button (=) |
| Post-processing: Point evaluation | Select Boundary 2 and expression $u$. Reports: Value: 0.861167, Expression: $u$, Boundary: 2 |

# Heat transfer equation

The steady state heat transfer equation is commonly met in engineering studies as the simplest PDE that is analytically solvable: Poisson's equation. Nevertheless, series solutions for complicated geometries may be intractable. The author has recently shown that some series so derived are purely asymptotic and poorly convergent [5]. Consequently, numerical solutions are likely to be better behaved than series expansions. Furthermore, any variation on the processes of heat transfer may destroy the analytic structure. In this section, we will consider the typical one-dimensional heat transfer problem in a slab of nonuniform conductivity and a distributed source that is differentially heated on the ends:

$$-\frac{d}{dx}\left(k\frac{dT}{dx}\right) = f(x)\,,$$

$$T|_{x=0} = 1 \quad T|_{x=1} = 0\,.$$

Table 9. Heat transfer in a nonuniform medium — Distributed source.

| | |
|---|---|
| Model Navigator | Select 1-D. COMSOL Multiphysics: Heat Transfer:Conduction: Steady state analysis. Set dependent variable: $u$ Select Element: Lagrange-Linear. OK |
| Draw Menu | Specify objects: Line. Coordinates pop-up menu. $x$: 0 1 name: interval OK |
| Physics Menu: Boundary settings | Select boundary selection 1 Set boundary condition: temperature; $T_0 = 1$ Select boundary selection 2 Set boundary condition; $T_1 = 0$. OK |
| Physics Menu: Subdomain settings | Select domain 1 Set $k = 1$; $Q = -x * (1 - x)$ Select Init tab; set $T(t_0) = 1 - x$. OK |
| Meshing | Click on triangle symbol to mesh |
| Solver | Click on the solve (=) button to solve |
| Post-processing: Data display | Specify $x = 0.5$ Value: 0.474097 $[K]$, Expression: $T$, Position: (0.5) |