ME-474 Numerical Flow Simulation

Comments on exercise: 1D steady diffusion

Fall 2023

Implement a FVM code in Matlab to solve a 1D steady-state heat conduction problem.
Equation:

$$\frac{\partial}{\partial x}\left(k(x)\frac{\partial T}{\partial x}\right) + S(x) = 0$$

Domain: $x \in [0, L]$, $L = 1$ m.
Assume the thermal conductivity is constant: $k = 400$ W/(K.m).

1. Consider Dirichlet boundary conditions: $T(0) = T_a = 300$ K, $T(L) = T_b = 320$ K. Assume the source term is constant: $S = S_c = 5000$ W/m^3.

   - Define a uniform grid of n nodes: $x_1 = 0$, $x_2 = \Delta x = L/(n-1) \ldots$, $x_n = L$. Start with $n = 21$.
     The usual Matlab command to create uniform grids is `linspace(0,L,n)`. One can also use the syntax `0:dx:L`.
   - Recall the discretized equation

     $$a_P T_P = a_W T_W + a_E T_E + b,$$

     or in vectorial form $\mathbf{AT} = \mathbf{b}$. Define the $n \times n$ matrix $\mathbf{A}$, and the $n \times 1$ right-hand side vector $\mathbf{b}$. Implement boundary conditions in equations 1 and n.
     Please note that the right notation to initialise a vector with zero entries is `zeros(n,1)` or `sparse(n,1)`, if you want to work with sparse matrices. The commands `zeros(n)` and `sparse(n)` generates `n`×`n` matrices. If you use central differencing as discretization scheme, the matrix A should be tri-diagonal. The first and last rows have to be replaced by the "Dirichlet" operator (i.e. the identity δ_{ij}).
   - Solve for $\mathbf{T}$ and plot $T(x)$.
     The use of the command `A\b` is advised since it allows to save computational time with respect to `inv(A)*b`.
   - Compare with the theoretical solution ($T'' = -S/k = cst \rightarrow$ quadratic $T(x)$):

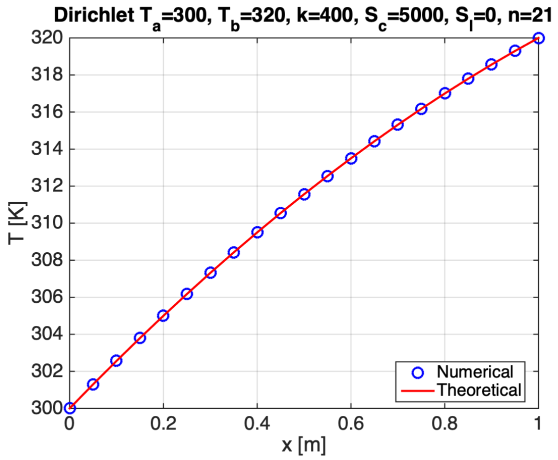
     $$T_{theo}(x) = \left(-\frac{S_c}{2k}\right)x^2 + \left(\frac{T_b - T_a}{L} + \frac{S_c L}{2k}\right)x + T_a.$$

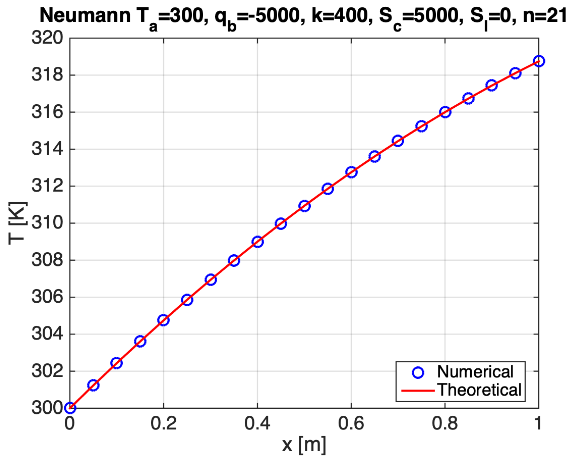
     This solution can be evaluated at the nodes of the grid built at the beginning, which makes it easier to compute the error (next question). It can also be evaluated on a finer grid, for instance for plotting purposes.
   - Check that the mean error

     $$e = \frac{1}{n}\sum_i |T_i - T_{theo,i}|$$

     is exactly zero whatever the value of n. Why?
     As explained below, this comes from the very specific situation we have here: the combination of a uniform grid and a quadratic solution.

     When discretizing the equation, we make two approximations: for the derivative $\partial T/\partial x$, and for the source term. With the central differencing scheme, the derivative is approximated as





$(\partial T/\partial x)_e \approx (T_E - T_P)/\delta x_{PE}$. Following the lecture slides, Taylor expansions at nodes P and E with respect to e read:

$$T_E = T_e + (x_E - x_e)\frac{\partial T}{\partial x} + \ldots + \frac{(x_E - x_e)^k}{k!}\frac{\partial^k T}{\partial x^k} + \ldots, \tag{1}$$

$$T_P = T_e + (x_P - x_e)\frac{\partial T}{\partial x} + \ldots + \frac{(x_P - x_e)^k}{k!}\frac{\partial^k T}{\partial x^k} + \ldots, \tag{2}$$

where the derivatives are evaluated in e. The difference of these two expressions gives

$$T_E - T_P = 0 + (x_E - x_P)\frac{\partial T}{\partial x} + \ldots + \frac{(x_E - x_e)^k - (x_P - x_e)^k}{k!}\frac{\partial^k T}{\partial x^k} + \ldots \tag{3}$$

On a uniform grid, the spacing is constant: $x_E - x_e = -(x_P - x_e) = \delta x$. Therefore we have:

$$(x_E - x_e)^k - (x_P - x_e)^k = \delta x^k - (-\delta x)^k = \left[1 - (-1)^k\right]\delta x^k = \begin{cases} 0 & \text{if } k \text{ is even,} \\ 2\delta x^k & \text{if } k \text{ is odd.} \end{cases} \tag{4}$$

So what remains in (3) is:

$$T_E - T_P = (x_E - x_P)\frac{\partial T}{\partial x} + \sum_{k\geq 3,\ \text{odd}} \frac{2\delta x^k}{k!}\frac{\partial^k T}{\partial x^k}. \tag{5}$$

If, in addition, the solution $T(x)$ is quadratic, all the derivatives $\partial^k T/\partial x^k$ are 0 for all $k \geq 3$, so finally we have without any approximation

$$T_E - T_P = (x_E - x_P)\frac{\partial T}{\partial x}. \tag{6}$$

In other words, in this very specific case, the central differencing scheme used to approximate $\partial T/\partial x$ is exact. A similar argument for the source term shows that the total error is zero.

2. Consider now the same Dirichlet boundary condition on the left, $T(0) = T_a = 300$ K, but a Neumann boundary condition on the right, $q_b = -k(\partial T/\partial x)_{x=L} = -5000$ W/m^2.

   - Modify the implementation of the boundary conditions. (It may be a good idea to save two different versions of your code.)
     The only difference with respect to the previous point consists of the implementation of the boundary condition.
   - Solve for $\mathbf{T}$ and plot $T(x)$.
   - Compare with the theoretical solution:

$$T_{theo}(x) = \left(-\frac{S_c}{2k}\right)x^2 + \left(\frac{S_c L - q_b}{k}\right)x + T_a.$$

- Check that the mean error per control volume is exactly zero whatever the value of n. Why?
  Same reason as in Q1.

3. Finally, come back to Dirichlet boundary conditions on both ends like in Q1, but assume now that the source term varies linearly with temperature:

$$S = S_c + S_l T.$$

Take for instance $S_c = 5000$ for the constant component, and $S_l = -100$ for the linear coefficient. Note that the integration of this source term over a control volume yields

$$\int_{x_w}^{x_e} S\,dx \approx \overline{S}\Delta x = (S_c + S_l T_P)\Delta x,$$

so now the constant right-hand side is $b = S_c \Delta x$, while the solution-dependent term $S_l T_P \Delta x$ goes into the diagonal coefficient $a_P T_P$.

- Modify the matrix $\mathbf{A}$ accordingly.
  It is sufficient to properly modify $i)$ the entries of b and $ii)$ the entries A_{ii} on the diagonal since, as we see from the previous formula, T is evaluated in the central point P.
- Solve for $\mathbf{T}$ and plot $T(x)$.
- Compare with the theoretical solution, that can be obtained as the sum of (i) a particular solution of the full equation $kT'' + S_l T = -S_c$, i.e. $T = -S_c/S_l$, and (ii) the general solution of the homogeneous equation $kT'' + S_l T = 0$, which is $T = c_1 e^{\mu x} + c_2 e^{-\mu x}$, with $\mu = \sqrt{-S_l/k}$, and c_1 and c_2 such that boundary conditions are satisfied, which yields:

$$T_{theo}(x) = -\frac{S_c}{S_l} + c_1 e^{\mu x} + c_2 e^{-\mu x}, \quad c_1 = \frac{T_b - \left(\frac{S_c}{S_l} + T_a\right) e^{-\mu L} + \frac{S_c}{S_l}}{e^{\mu L} - e^{-\mu L}}, \quad c_2 = T_a + \frac{S_c}{S_l} - c_1.$$

- Observe that the mean error per control volume is not zero. Why? How does it decrease with n? (Plot the mean error as a function of n in log-log scale.)
  In this case the solution does not have higher-order derivatives that vanish, so the approximation is not exact.
  When using a scheme of order M, the mean error in a log-log plot is represented by a straight line of slope M. Here the scheme should be of order 2, so the error should decrease like:

$$e \sim (\Delta x)^2 \sim 1/n^2 \quad \Rightarrow \quad \log(e) \sim -2\log(n).$$

  This is indeed what is observed in the figure below (right panel), where the error is plotted for $n = 4, 8, 16, 32, 64$ in log-log scale.