Homework set 3

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1 Problem 1 - The Thomas algorithm - Tri-diagonal matrix solver

In class you have seen the Thomas algorithm, in this homework, you will implement the algorithm and use it to solve some simple tri-diagonal linear systems.

(a) Write a function **thomas_TRDMA.m** that takes 5 input parameters: the 3 diagonals of the matrix in vector format, another vector for the right-hand side of the linear system and finally the size of the linear system to solve for. *Advice: to test your function try to solve the trivial system*

$$\mathcal{I}x = c, \tag{1}$$

where $\mathcal{I}$ is the identity square matrix (use here a 4 by 4 matrix), x the vector to solve for and $c = (1, 2, 3, 4)$. Show your result and discuss if it is correct.

(b) Use **thomas_TRDMA.m** to solve the following system

$$Ax = b, \tag{2}$$

with x and b being vectors with 10 elements, and $b = (1, 2, \ldots, 10)$, and A is a 10 by 10 matrix with lower and upper diagonal values that are equal to the line they occupy in the matrix and the diagonal of A, $A_{ii} = 40$. Use a timer (see discussion in class or check the help in Matlab) to measure the time it took your computer to solve the system and compare it with the time it takes when you use the *inv* function (inverts a matrix) with Matlab. Check that the two solutions are identical, print the results for both calculations and the calculation time. If possible, write down the specs of the computer that you used (processor, RAM memory).

Turn in a copy of **thomas_TRDMA.m** and your results.

2 Problem 2 - The steady diffusion equation

Here you will solve for the following equation

$$\frac{d^2T}{dx^2} = S(x), \tag{3}$$

where $S(x)$ is a source term. Write a script (driver) **SteadyDiff.m** that requires inputs from the user, namely the size of the domain L and the number of gridpoints $N = L/dx$. After entering these informations, the script should read the source function $S(x)$ from a function file **source.m** which builds a vector V of dimension N

$$V = (S(dx), S(2dx), \dots, S(Ndx)). \tag{4}$$

After this, the script should use a modified version of the Thomas algorithm you wrote above that sends two more input variables: T_l and T_r, respectively the left and right boundary conditions (equivalent to positions $x = 0$ and $x = L + dx$. Make sure that the new version of the Thomas algorithm **thomasMod.m** takes these two boundary conditions into account during the solution process (*HINT: include these boundary conditions into the right-hand side vector b of the system $Ax = b$.*
Solve the following problem: $S(x) = 2x$, $T_l = 1$ and $T_r = 2$, derive the analytical solution and compare it graphically with the numerical solution you obtained. Print your functions and script, the results (plot with analytical and numerical solutions) and the derivation of the analytical solution.

3 Problem 3 - Chemical reactions