

Programming assignment III
ME685A – APPLIED NUMERICAL METHODS

6th April 2022

Discretize the unsteady 1D diffusion equation for species concentration in a slab with radioactive decay on a grid of N nodes. Adopt the FTCS implicit method. The applicable governing equation with IC/BC is:

$$\begin{aligned}\frac{\partial T}{\partial t} &= \alpha \frac{\partial^2 T}{\partial x^2} - \lambda T \quad 0 < x < L; \quad t > 0 \\ t = 0, \quad T(x, 0) &= 0 \\ x = 0, \quad T(0, t) &= 1; \quad x = L, \quad T(L, t) = 0\end{aligned}$$

Solve the system of algebraic equations arising from FTCS using the successive substitution formula (Gauss-Seidel method). Also derive the analytical steady state solution.

Weightage of numerical solution 90% and analytical 10%

Show results for the number of points $N=101$. For definiteness, set $\alpha = 1$; $\lambda = 9$; $L = 1$. Choose a time step of 0.005 and perform time integration to at least $t=1$. The program output should comprise the left wall concentration gradient as well as concentration at the mid-point of the slab, as a function of time. Compare the numerical solution with the analytical (steady state).

Summarize your results in the form of a report. The zipped file should contain the pdf of your report and the computer program.

Hint: The full analytical solution is derived by first introducing a new dependent variable

$T(x, t) = \phi(x, t) \exp(-\lambda t)$. Hence, with $\alpha = 1$; $\lambda = 9$; $L = 1$ we get

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} \quad 0 < x < 1; \quad t > 0$$

$$t = 0, \quad \phi(x, 0) = 0$$

$$x = 0, \quad \phi(0, t) = \exp(\lambda t); \quad x = 1, \quad \phi(1, t) = 0$$

The analytical solution is obtained using Duhamel's theorem.

Hence we get the following results: { ϕ and ϕ_H are intermediate solutions. }

$$\phi_H(x, t) = (1 - x) + \sum_{n=1}^{\infty} c_n \sin(n\pi x) \exp(-n^2 \pi^2 t) \quad \text{with} \quad c_n = \frac{\int_0^1 (x-1) \sin n\pi x dx}{\int_0^1 \sin^2 n\pi x dx} \quad \text{Consider 100 terms in } \sum_{n=1}^{\infty} c_n.$$

$$\phi(x, t) = \int_0^t \exp(\lambda \tau) \frac{\partial}{\partial t} [\phi_H(x, t - \tau)] d\tau \quad \text{and}$$

$$T(x, t) = \int_0^t \exp(-\lambda(t - \tau)) \frac{\partial}{\partial t} [\phi_H(x, t - \tau)] d\tau$$

$\frac{\partial}{\partial t} [\phi_H(x, t - \tau)]$ is evaluated as $\frac{\partial \phi_H(x, t)}{\partial t}$
followed by 't' replaced by 't - \tau'.

This is the required analytical solution for $T(x, t)$. The steady state solution is much simpler and is obtained by solving the ODE

$$\begin{aligned}0 &= \frac{d^2 T}{dx^2} - \lambda T \quad 0 < x < L; \quad t > 0 \\ x = 0, \quad T(0, t) &= 1; \quad x = L, \quad T(L, t) = 0\end{aligned}$$