On The Discretization Time-step in the Finite Element Theta-method of the Two-dimensional Discrete Heat Equation

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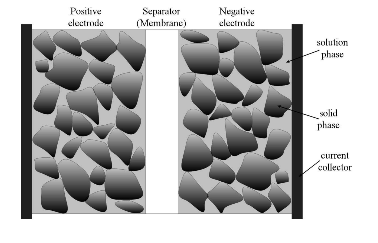
Outline

Motivation

- The Proton exchange membrane fuel cells (PEMFC) are electrochemical conversion devices that produce electricity from fuel and an oxidant.
- The the membrane would dry on higher temperatures!
- Since the heat produced in fuel cells appearing on a specified side of cell, we need to apply different boundary conditions on different sides of the two dimensional mathematical model.



Problem

Two-dimensional classical diffusion problem: **The heat conduction equation**

The general form of the equation on $\Omega \times (0,T)$, where $\Omega := [0,1] \times [0,1]$, is

$$\begin{aligned} c\frac{\partial u}{\partial t} &= \kappa \nabla^2 u, \quad (x,y) \in \Omega,\ t \in (0,T), \\ u|_{\Gamma_D} &= \tau,\ \left.\frac{\partial u}{\partial n}\right|_{\Gamma_N} = 0,\ t \in [0,T) \\ u(x,y,0) &= u_0(x,y),\ (x,y) \in \Omega, \end{aligned} \tag{1}$$

Γ_N : Neumann boundary condition ($x=0$ or $x=1$ or $y=1$),

Γ_D : Dirichlet boundary condition was applied ($y=0$)

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Numerical solution is needed $\rightarrow$ Which time step size of the finite element theta-method can be used to retain the physical characteristics of the solution?

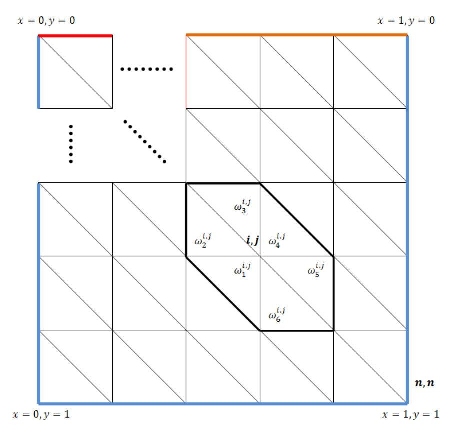
Semi-Discretization

We seek the spatially discretized temperature u_d in the form:

$$u_d(x,y,t) = \sum_{i,j=0}^{n} \phi_{i,j}(t) N_{i,j}(x,y), \tag{2}$$

where $N_{i,j}(x)$ are the following shape functions:

$$N_{i,j}(x) := \begin{cases} 1 - \frac{1}{h}(x_i - x) - \frac{1}{h}(y_j - y), & \text{if } (x,y) \in \omega_1^{i,j} \\ 1 - \frac{1}{h}(x_i - x), & \text{if } (x,y) \in \omega_2^{i,j} \\ 1 + \frac{1}{h}(y_j - y), & \text{if } (x,y) \in \omega_3^{i,j} \\ 1 + \frac{1}{h}(x_i - x) + \frac{1}{h}(y_j - y), & \text{if } (x,y) \in \omega_4^{i,j} \\ 1 + \frac{1}{h}(x_i - x), & \text{if } (x,y) \in \omega_5^{i,j} \\ 1 - \frac{1}{h}(y_j - y), & \text{if } (x,y) \in \omega_6^{i,j} \end{cases} \tag{3}$$



The equilateral triangle grid on the analysed domain

By redistributing the indices, the following equations draw up:

$$\sum_{i,k=0}^{n} \phi_{i,k}^{'}(t) \int_{\Omega} cN_{i,k}N_{j,l}dydx +$$
$$\sum_{i,k=0}^{n} \phi_{i,k}(t) \int_{\Omega} \kappa \left(\frac{\partial N_{i,k}}{\partial x}\frac{\partial N_{j,l}}{\partial x} + \frac{\partial N_{i,k}}{\partial y}\frac{\partial N_{j,l}}{\partial y} \right) dydx = 0, \quad (4)$$
$$j = 1, 2 \ldots n, \; l = 0, 1 \ldots n.$$

Let $\underline{K}, \underline{M} \in \mathbf{R}^{(n+1)\times n^3}$ denote the so-called stiffness and mass matrices, respectively, defined by:

$$(\underline{K_{k,l}})_{i,j} = \int_{\Omega} \kappa \left(\frac{\partial N_{i,k}}{\partial x}\frac{\partial N_{j,l}}{\partial x} + \frac{\partial N_{i,k}}{\partial y}\frac{\partial N_{j,l}}{\partial y} \right) dydx, \quad (5)$$
$$(\underline{M_{k,l}})_{i,j} = \int_{\Omega} cN_{i,k}N_{j,l}dydx. \quad (6)$$

Finite-element Theta Method

(4) can be expressed as:

$$\underline{M}\,\underline{\Phi}' + \underline{K}\,\underline{\Phi} = 0, \tag{7}$$

Discretization:

- Space $\rightarrow$ Linear finite element method
- Time $\rightarrow$ Theta-method

$$\underline{M}\frac{\underline{\Phi}^{m+1} - \underline{\Phi}^{m}}{\Delta t} + \underline{K}\left(\Theta\underline{\Phi}^{m+1} + (1-\Theta)\underline{\Phi}^{m}\right) = 0. \tag{8}$$

where Θ is related to the numerical method and it is an arbitrary parameter on the interval $[0, 1]$.

$\Theta = 0.5 \rightarrow$ Crank-Nicolson implicit method.

Analysis of FEM Equation

Let Φ_i denote the transpose of the temperature vector at the i-th row of the discretization of Ω, namely $\Phi_i = (\Phi_{i,0}, \Phi_{i,1}, \ldots, \Phi_{i,n})^T$. It is worth emphasizing that, there could be a discontinuity in the initial conditions at $y = 0$. We investigate the condition under which the first iteration, denoted by Φ=Φ^1, results in non-negative approximation.

First we put $u_0(x) = 0$, which yields $\Phi_i^0 = 0$, $(i = 1, 2, ..., n)$.
Considering the fact that the matrices of equation (8) are block tridiagonal matrices the following system can be obtained:

$$\begin{aligned} A\Phi_0 + B\Phi_1 + C\Phi_2 &= 0 \\ A\Phi_1 + B\Phi_2 + C\Phi_3 &= 0 \\ &\dots \\ A\Phi_{n-2} + B\Phi_{n-1} + C\Phi_n &= 0 \\ A\Phi_{n-1} + D\Phi_n &= 0 \end{aligned}$$

We seek the solution in the form

$$\Phi_i = Z_i \Phi_0, \ i = 0, 1, ..., n. \tag{9}$$

Obviously, Z_0 is the n-by-n indentity matrix. Φ_n can be expressed as

$$\Phi_n = -D^{-1} A Z_{n-1} \Phi_0, \tag{10}$$

which implies that

$$Z_n = -D^{-1} A Z_{n-1} = X_{n-1} Z_{n-1}, \tag{11}$$

where

$$X_{n-1} = -D^{-1} A. \tag{12}$$

In the next step, Z_{n-1} can be expressed applying (11), and then for the i-th equation the following relation holds:

$$Z_i = -\left(B + C X_i\right)^{-1} A Z_{i-1} = X_{i-1} Z_{i-1}, \ i = 1, 2, ..., n-1, \tag{13}$$

where

$$X_{i-1} = -\left(B + C X_i\right)^{-1} A, \ i = n-1, n-2, ..., 1. \tag{14}$$

We obtained the following statement.

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The relation $\Phi_i \geq 0$ holds only under the condition $Z_i \geq 0$. From (13) we can see that it is equivalent to the non-negativity of X_i for all $i = 0, 1, ..., n-1$.

Characteristics

Using the one-step iterative method to the discretization of (7) the following system of linear algebraic equations is obtained:

$$P_1\Phi^{m+1} = P_2\Phi^m, \; m = 0, 1, \dots, \tag{15}$$

where $P_1 = M + \Delta t\Theta K$, $P_2 = M - \Delta t(1-\Theta)K$. It is clear that for all Φ^{m+1} to be non-negative, the non-negativity of the following matrix is required:

$$P = P_1^{-1}P_2 \tag{16}$$

The sufficient conditions of the non-negativity of P are the following:

$$P_1^{-1} \geq 0 \;\text{ and }\; P_2 \geq 0. \tag{17}$$

For P_2 it is easy to give a condition that guarantees its non-negativity. By analyzing the elements of the matrix. The following condition can be obtained:

$$\frac{h^2 c}{2\Delta t} - 4\kappa(1-\Theta) \geq 0, \tag{18}$$

which is equivalent to the condition

$$\Delta t \leq \frac{h^2 c}{8(1-\Theta)\kappa}. \tag{19}$$

It is not possibile to obtain a sufficient condition for the non-negativity of the matrix P_1^{-1} by the so-called M-Matrix method. It follows from the fact that P_1 contains some positive elements in its offdiagonal. Therefore, a sufficient condition for the inverse-positivity of P_1 is obtained by Lorenz.

Lemma

(Lorenz) Let A be an n-by-n matrix, denote A_d and A^- the diagonal and the negative offdiagonal part of the matrix A, respectively. Let $A^- = A^z + A^s = (a_{ij}^z) + (a_{ij}^s)$. If

$$a_{ij} \leq \sum_{k=1}^{n} a_{ik}^z a_{kk}^{-1} a_{kj}^s, \ \forall a_{ij}, i \neq j, \tag{20}$$

then A is a product of two M-matrices, i.e., A is monoton.

We could analyse matrix P_1 with the theorem if it is decomposed into the diagonal part, the positive offdiagonal part, the upper triangular and lower triangular negative parts. All the conditions of the theorem are satisfied if:

$$\frac{1}{12} \leq \frac{\left(\frac{1}{12} - \kappa\frac{\Delta t}{h^2 c}\right)^2}{\frac{1}{2} + 4\kappa\frac{\Delta t}{h^2 c}}, \tag{21}$$

which implies the lower bound

$$\frac{h^2 c}{12\Theta\kappa}\left(3 + \sqrt{14}\right) \leq \Delta t \tag{22}$$

Summary

The following statement is proven.

Theorem

Let us assume that the conditions

$$\frac{h^2 c}{12\Theta\kappa}\left(3+\sqrt{14}\right) \le \Delta t \le \frac{h^2 c}{8(1-\Theta)\kappa}, \qquad (23)$$

hold. Then for the problem (1) *with arbitrary non-negative initial condition the linear finite element method results in a non-negative solution on any time level.*

Thank you for your attention!

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