

## Finite volume schemes for multilayer diffusion

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### HIGHLIGHTS

- Finite volume method for layered diffusion problems is developed.
- Proposed method is applicable to general boundary/interface conditions.
- Theoretical analysis (stability and convergence) of the schemes is presented.
- Finding: interface conditions can lead to more restrictive stability conditions.
- Presented numerical results confirm the theoretical analysis.

### ARTICLE INFO

#### Article history:

Received 20 November 2017

Received in revised form 18 April 2018

#### Keywords:

Multilayer diffusion

Finite volume scheme

Stability and convergence

Gershgorin circle theorem

Interface conditions

### ABSTRACT

This paper focusses on finite volume schemes for solving multilayer diffusion problems. We develop a finite volume method that addresses a deficiency of recently proposed finite volume/difference methods, which consider only a limited number of interface conditions and do not carry out stability or convergence analysis. Our method also retains second-order accuracy in space while preserving the tridiagonal matrix structure of the classical single-layer discretisation. Stability and convergence analysis of the new finite volume method is presented for each of the three classical time discretisation methods: forward Euler, backward Euler and Crank–Nicolson. We prove that both the backward Euler and Crank–Nicolson schemes are always unconditionally stable. The key contribution of the work is the presentation of a set of sufficient stability conditions for the forward Euler scheme. Here, we find that to ensure stability of the forward Euler scheme it is not sufficient that the time step  $\tau$  satisfies the classical constraint of  $\tau \leq h_i^2/(2D_i)$  in each layer (where  $D_i$  is the diffusivity and  $h_i$  is the grid spacing in the  $i$ th layer) as more restrictive conditions can arise due to the interface conditions. The paper concludes with some numerical examples that demonstrate application of the new finite volume method, with the results presented in excellent agreement with the theoretical analysis.

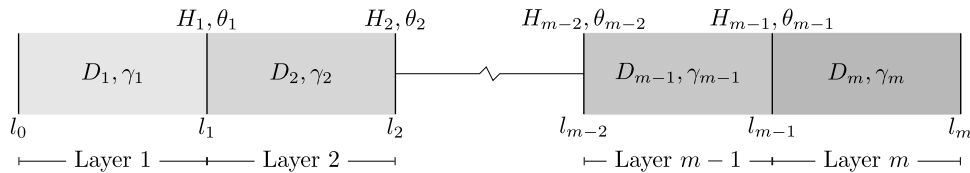
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### 1. Introduction

Many industrial, environmental and biological problems involve diffusion processes across layered materials. For example, heat conduction in composites [1–3], tumour growth across the white and grey matter components of the brain [4,5], contaminant transport across layered soils [6,7] and thermal conduction through skin layers during burning [8] all involve multilayer diffusion processes. Additionally, layered diffusion is of interest to the applied mathematics community as it can be thought of as a simple example of a multiscale problem when the number of layers is large [9,10]. These applications have led to a recent flourish in research activity focussed on analytical and numerical methods for solving mathematical models of multilayer diffusion [9,11–16].

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**Fig. 1.1.** Schematic diagram of a layered medium consisting of  $m$  layers. The diffusion coefficient  $D_i$  and conductivity coefficient  $\gamma_i$  are constant in each layer ( $i = 1, \dots, m$ ) with the contact transfer and partition coefficients between the  $i$ th and  $(i + 1)$ th layers denoted by  $H_i$  and  $\theta_i$  respectively.

This paper focusses on the numerical solution of the multilayer diffusion problem described as follows. Consider a diffusion process defined on an interval  $[l_0, l_m]$  partitioned into  $m$  distinct layers, such that  $l_0 < l_1 < \dots < l_{m-1} < l_m$ , where  $x = l_i$  ( $i = 1, \dots, m - 1$ ) specifies the location of the interface between the  $i$ th and  $(i + 1)$ th layers (see Fig. 1.1). The resulting domain is denoted  $[l_0, l_1, \dots, l_{m-1}, l_m]$ . In this work, we define a linear diffusion equation on each layer together with general initial and boundary conditions:

$$\frac{\partial u_i}{\partial t} = D_i \frac{\partial^2 u_i}{\partial x^2}, \quad l_{i-1} < x < l_i, \quad t > 0, \tag{1.1}$$

$$u_i(x, 0) = f_i(x), \tag{1.2}$$

$$a_L u_1(l_0, t) - b_L \frac{\partial u_1}{\partial x}(l_0, t) = c_L, \tag{1.3}$$

$$a_R u_m(l_m, t) + b_R \frac{\partial u_m}{\partial x}(l_m, t) = c_R, \tag{1.4}$$

where  $u_i(x, t)$  is the solution in the  $i$ th layer at position  $x$  and time  $t$ ,  $D_i > 0$  is the diffusion coefficient in the  $i$ th layer,  $f_i(x)$  specifies the initial solution in the  $i$ th layer at position  $x$ , and  $a_L, b_L, c_L, a_R, b_R$  and  $c_R$  are non-negative constants satisfying  $a_L + b_L > 0$  and  $a_R + b_R > 0$ . We neglect the special case of Neumann conditions on both boundaries (i.e.  $a_L = a_R = 0$ ). A unique feature of multilayer problems are the internal boundary conditions that apply at the interfaces between adjacent layers. To close the problem (1.1)–(1.4), at each interface,  $x = l_i$  ( $i = 1, \dots, m - 1$ ), a pair of interface conditions is imposed, which we assume are chosen from one of the following four types:

(i) Type I:

$$u_i(l_i, t) = u_{i+1}(l_i, t), \tag{1.5}$$

$$D_i \frac{\partial u_i}{\partial x}(l_i, t) = D_{i+1} \frac{\partial u_{i+1}}{\partial x}(l_i, t). \tag{1.6}$$

(ii) Type II:

$$D_i \frac{\partial u_i}{\partial x}(l_i, t) = H_i(u_{i+1}(l_i, t) - u_i(l_i, t)), \tag{1.7}$$

$$D_{i+1} \frac{\partial u_{i+1}}{\partial x}(l_i, t) = H_i(u_{i+1}(l_i, t) - u_i(l_i, t)). \tag{1.8}$$

(iii) Type III:

$$u_i(l_i, t) = u_{i+1}(l_i, t), \tag{1.9}$$

$$\gamma_i \frac{\partial u_i}{\partial x}(l_i, t) = \gamma_{i+1} \frac{\partial u_{i+1}}{\partial x}(l_i, t). \tag{1.10}$$

(iv) Type IV:

$$u_i(l_i, t) = \theta_i u_{i+1}(l_i, t), \tag{1.11}$$

$$D_i \frac{\partial u_i}{\partial x}(l_i, t) = D_{i+1} \frac{\partial u_{i+1}}{\partial x}(l_i, t). \tag{1.12}$$

Each of the four types of interface conditions (1.5)–(1.12) models different physical processes at the interfaces and as a result finds application to different industrial, environmental and biological problems. Both Type I and Type III conditions assume that the  $i$ th and  $(i + 1)$ th layers are in perfect contact, that is, the solution is continuous across the  $i$ th interface. The difference is that Eq. (1.6) imposes continuity of the diffusive flux across the interface, whereas Eq. (1.10) allows for a more general formulation, where the flux depends on an arbitrary coefficient  $\gamma_i > 0$  instead of the diffusion coefficient  $D_i$ . The latter interface condition is useful in heat conduction problems, for example, where the diffusion coefficient is the ratio of the thermal conductivity to the volumetric heat capacity, as Eq. (1.10) allows one to impose continuity of the heat flux as

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