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Integral equation formulation of an unsteady diffusion–convection equation with variable coefficient and velocity

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ABSTRACT

In this paper we present an integral equation formulation for the time dependent diffusion–convection equation with variable coefficient and velocity with sources. The formulation is based on usage of the steady fundamental solution of the convection–diffusion equation. For a known velocity and coefficient fields, which may change with location and time, the formulation avoids the usage of the gradient of the unknown field function and thus avoids making the problem nonlinear. Two discretization approaches are proposed and compared: a standard single domain boundary–domain element technique and a domain decomposition approach. The validity of the formulation and comparison of discretization approaches is preformed on several challenging test cases. Mesh convergence is reported and the advantages and disadvantages of both approaches are examined.

1. Introduction

Convective and diffusive transport processes occur frequently in nature and engineering. Since fluid flow is in general an unsteady three-dimensional phenomenon, the transport processes taking place in such flows are governed by a velocity field, which changes with time and location. Furthermore, the transport coefficient (i.e. diffusivity in the case of mass transfer, heat conductivity in the case of heat transfer or viscosity in the case of momentum transfer) may also change with time and location. The change may be due to physical processes, such as a change in fluid temperature or pressure. Changes in diffusivity may also be due to the use of modelling of different physical phenomena as diffusion type processes with the introduction of a model based diffusivity. A prominent example of such modelling is the Reynolds averaged turbulence model, which introduces time and spatially varying turbulent viscosity. The turbulent viscosity is added to molecular viscosity in the convection–diffusion momentum transfer equation. In many disciplines, like environmental flows, soil physics, petroleum engineering, chemical engineering and biosciences, diffusive and convective processes with variable coefficients occur. There are many other application areas, where variable diffusion coefficients are used, such as, for example, in lithium ion battery electrodes (Renganathan and White [1]).

Since the convection–diffusion type equations govern many physical processes, many researchers worked on finding new solution methods. Most of the work was done with constant coefficients. Recently, Dehghan [2] proposed a numerical method for the solution of the three-dimensional advection–diffusion equation. Pudykiewicz [3] derived a finite volume algorithm for the solution of the reaction–advection–diffusion equation on the sphere. Sakai and Kimura [4] used a spectral method to solve a nonlinear two-dimensional unsteady advection–diffusion equation, which they transformed into a linear equation. Remešikova [5] proposed an operator splitting scheme for the numerical solution of two-dimensional convection–diffusion–adsorption problems.

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Kumar et al. [6] derived analytical solutions for the one-dimensional advection–diffusion equation with variable coefficients in a longitudinal finite initially solute free domain. Mikhailov [7] considered a solution of the heat equation with a time dependent coefficient. Ang et al. [8] used the boundary element method for a second order elliptic partial differential equation with variable coefficients. Similarly, Grzhibovskis et al. [9] considered a Dirichlet problem for the linear second order elliptic PDE in a bounded domain with variable coefficient. A boundary–domain integral equation was used, accelerated by the H-matrix/ACA technique. Several other authors also considered variable coefficient diffusion and Helmholtz equations in non-homogeneous media [10–16].

In this paper we propose an integral formulation, which leads to an efficient solution of unsteady diffusion–convection problems with variable velocity field and coefficient. This work is based on the formulation proposed by Ravnik and Škerget [17] for steady diffusion–convection problems. The gradient of the unknown field function is not included in the final integral formulation. Instead, the gradient of the coefficient is needed and thus, the final integral equation includes only the unknown function on the boundary and in the domain and its flux on the boundary. The proposed equation is linear and after discretization requires only a single solution of a system of linear equations to obtain the solution.

2. Governing equation

Let us consider a domain Ω in $\mathbb{R}^3$ with boundary Γ. The domain is filled with an incompressible fluid. Let $\vec{r}$ be a vector representing a point in the domain and let $\vec{v}$ be the fluid velocity. An unknown field function, u, which is subjected to convective and diffusive processes in the domain, is governed by the following PDE:

$$\frac{\partial u}{\partial t} + \vec{v}(\vec{r},t) \cdot \vec{\nabla} u = \vec{\nabla} \cdot \left(\alpha(\vec{r},t)\vec{\nabla} u\right) + f(\vec{r},t), \quad \vec{r} \in \Omega, \tag{1}$$

with the following Dirichlet and/or Neumann type boundary conditions

$$\begin{aligned} u(\vec{r},t) &= \overline{u}(\vec{r},t), \quad \vec{r} \in \Gamma_D, \\ \vec{n} \cdot \vec{\nabla} u(\vec{r},t) &= q(\vec{r}) = \overline{q}(\vec{r},t), \quad \vec{r} \in \Gamma_N, \end{aligned} \tag{2}$$

where Γ_D and Γ_N are the Dirichlet and Neumann parts of the boundary with $\Gamma = \Gamma_D \cup \Gamma_N$. Boundary conditions vary with time, while the initial conditions are

$$u(\vec{r},0) = u_0. \tag{3}$$

The fluid is incompressible, thus $\vec{\nabla} \cdot \vec{v} = 0$ and the fluid velocity varies in space and in time. The diffusion coefficient, α, in the domain is isotropic, time dependent and non-homogeneous, thus $\alpha(\vec{r},t)$ is a function of the location and time. Furthermore, there are sources $f(\vec{r},t)$ in the domain, which also vary in space and time.

3. Integral representation

The governing equation (1) may be recast into an integral form using the boundary–domain integral method (Škerget et al. [18]). The method relies on the fact that a fundamental solution of the steady diffusion–convection problem exists. It is defined by (Driessen [19])

$$\alpha_0 \nabla^2 u^\star + \vec{v}_0 \cdot \vec{\nabla} u^\star = -\delta(\vec{r},\vec{\xi}), \tag{4}$$

where α_0 and $\vec{v}_0$ are the constant parts of the transport coefficient and velocity and $\vec{\xi}$ is a source (collocation) point. Eq. (4) in 3D has the following fundamental solution:

$$u^\star(\vec{r},\vec{\xi}) = \frac{1}{4\pi|\vec{r}-\vec{\xi}|\alpha_0} \exp\left(\frac{\vec{v}_0 \cdot (\vec{r}-\vec{\xi}) - v_0|\vec{r}-\vec{\xi}|}{2\alpha_0}\right), \tag{5}$$

where $v_0 = |\vec{v}_0|$ and its gradient is

$$\vec{\nabla} u^\star(\vec{r},\vec{\xi}) = \left[\left(\frac{1}{|\vec{r}-\vec{\xi}|} + \frac{v_0}{2\alpha_0}\right)\frac{\vec{r}-\vec{\xi}}{|\vec{r}-\vec{\xi}|} - \frac{\vec{v}_0}{2\alpha_0}\right] u^\star(\vec{r},\vec{\xi}). \tag{6}$$

The variable coefficient and the velocity field are decomposed into constant and variable parts as follows:

$$\alpha(\vec{r}) = \alpha_0 + \alpha', \qquad \vec{v}(\vec{r}) = \vec{v}_0 + \vec{v}', \tag{7}$$

where α' and $\vec{v}'$ are the variable parts.

At time t for a time step Δt the backward Euler finite difference approximation is used to approximate the time derivative as

$$\frac{\partial u}{\partial t} = \beta_1 u + \beta_2 u^c \tag{8}$$

where $\beta_1 = \frac{1}{\Delta t}$ and $\beta_2 = -\frac{1}{\Delta t}$. The u is the function in the next time step and u^c is the function in the current time step.