Applied Numerical Mathematics 74 (2013) 62–82

Contents lists available at ScienceDirect

Applied Numerical Mathematics

www.elsevier.com/locate/apnum

High resolution methods for scalar transport problems in compliant systems of arteries

M. Tavelli, M. Dumbser *, V. Casulli

Laboratory of Applied Mathematics, Department of Civil, Environmental and Mechanical Engineering, University of Trento, Via Mesiano 77, 38123 Trento, TN, Italy

ARTICLE INFO

Article history:
Received 16 March 2013
Received in revised form 24 June 2013
Accepted 28 June 2013
Available online 26 August 2013

Keywords:
Scalar transport
Advection–diffusion equation
Compliant arterial systems
Unstructured staggered grids
Semi-implicit finite volume method

ABSTRACT

In this paper a new semi-implicit high resolution scheme for the simulation of advection–diffusion problems in compliant arterial systems is proposed. Such transport problems are not only of great importance for the modeling of drug delivery processes, but also for the simulation of continuous processes occurring in the human body such as the exchange of oxygen, carbon dioxide, nutrients and toxics. Assuming cylindrical geometry and axially symmetric blood flow, a finite volume scheme for scalar transport on unstructured staggered grids is derived. It is shown how both mass conservation and maximum principle can be assured by the present method. Since the discrete maximum principle imposes a CFL type restriction on the time step, the scalar transport equation is solved using a consistent local time-stepping approach in order to not affect the unconditional stability of the underlying semi-implicit scheme for the hydrodynamics. It is a key feature of the present approach that the radial profiles of axial velocity and scalar concentration are computed directly from *first principles* and that no heuristic model for the velocity profile is needed as in classical one-dimensional approaches, which are still frequently used for the simulation of artery trees. The knowledge of radial velocity and concentration gradients is fundamental for the exchange processes happening across the vessel walls. The accuracy of the proposed approach is validated on one- and two-dimensional test problems with exact solution. An example for scalar transport in a model artery tree with 55 branches rounds off the numerical test problems discussed in this paper.

1. Introduction

The modeling of blood flow in human arterial systems is a very challenging and highly interdisciplinary topic (see, e.g., [32,24,36]) that requires not only expertise in numerical analysis and applied mathematics, but it also requires the input of other scientific disciplines such as fluid and solid mechanics, human anatomy and physiology, as well as medical imaging. Very often, embedded multi-scale methods are used, where the main part of the artery network is simulated using rather simple and computationally efficient 1D models that are then locally enriched by multi-dimensional models in important parts of the system like particular junctions of larger blood vessels or the aortic arc, see, e.g., [17,35,21,22,36,23].

Once the velocity field and the vessel profile have been computed, one is often interested in the transport and exchange of additional scalar quantities, such as the concentration of drugs, oxygen, toxins, contrast agents, or other passive constituents [20,48]. The governing PDE of such advection–diffusion processes can be written either in conservation form or in a non-conservative way, where mass conservation follows immediately from the first formulation and a general maximum

* Corresponding author.
E-mail address: michael.dumbser@unitn.it (M. Dumbser).

0168-9274/$36.00
http://dx.doi.org/10.1016/j.apnum.2013.06.009

principle from the second one. At the discrete level, one would require from the numerical scheme to fulfill at the same time the conservation property as well as a discrete maximum principle.

Based on the mass-conservative semi-implicit method proposed in [10] for the simulation of the hydrodynamics in compliant axially symmetric arterial systems, in this paper the advection–diffusion equation of a passive scalar is discretized in such a fashion that the resulting numerical solution actually satisfies both properties, mass conservation and the maximum principle for the concentration of the advected scalar. A high resolution version of the transport scheme is constructed by using classical TVD flux limiters.

This problem, which was studied in a different context in [13], will be investigated in the present paper for compliant arterial systems. Recently, an efficient semi-implicit method for the simulation of axially symmetric blood flow in compliant vessels in one and two dimensions has been provided in [10]. The semi-implicit numerical scheme derived there for the hydrodynamics has been also applied successfully to environmental free surface flow problems in two and three space dimensions in a series of papers, see, e.g., [7,9,12,40,28,3]. Furthermore, a method for the scalar transport compatible with the blood flow equations will be derived in this paper in a similar way as shown in [13] for free surface hydrodynamics. The resulting method is conservative and satisfies the maximum principle.

The paper is organized as follows: for the sake of clarity the method is first presented for the case of one-dimensional arterial networks in Section 2 and is subsequently extended to the two-dimensional axially symmetric case in Section 3. Numerical test problems are presented in Section 4 and the paper closes with some concluding remarks in Section 5.

2. A one-dimensional transport model

The momentum equation for one-dimensional hydrostatic flows (see, e.g., [2] and [47]) is given in non-conservative form by

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = -\frac{\partial p}{\partial x} - \frac{4\nu}{R^2}u. \tag{1}$$

Here, x and $u(x,t)$ are the axial direction and the axial velocity, respectively; t is the time; $p(x,t)$ is the unknown normalized pressure; $\nu \geqslant 0$ is the kinematic viscosity of the fluid; $R(x,t)$ is the unknown arterial radius. Moreover, the continuity equation for one-dimensional flow through compliant tubes with variable cross section reads

$$\frac{\partial A}{\partial t} + \frac{\partial (Au)}{\partial x} = 0, \tag{2}$$

where $A = \pi R^2$ is the cross-sectional area that is linked to the pressure p by a so-called *equation of state*. Throughout this paper the vessel walls are described by an elastic ring theory that leads to the following equation of state (law of Laplace):

$$p = p_{ext} + \beta(R - R_0), \tag{3}$$

where p_{ext} is a given external pressure, β is a rigidity coefficient and R_0 is the equilibrium radius (see, e.g., [47]). The constants R_0 and β can be obtained for example by in vivo measurements and the solution of inverse problems, as explained in [33]. The mass conservation of a passively transported scalar variable is expressed by the following additional differential equation:

$$\frac{\partial (AC)}{\partial t} + \frac{\partial (uAC)}{\partial x} = \frac{\partial}{\partial x}\left(\Gamma^x A \frac{\partial C}{\partial x}\right), \tag{4}$$

where $C(x,t)$ denotes the sectionally averaged concentration of the transported substance and $\Gamma^x \geqslant 0$ is a given horizontal mass-diffusivity coefficient.

2.1. Staggered unstructured grid

The arterial system consists of interconnected branches, each of which is discretized according to [10] by a set of non-overlapping computational elements. Hence, the computational domain is discretized by N_s elements in axial direction, in the following also called segments synonymously. The segments have in general a non-uniform length Δx_j for $j = 1, \ldots, N_s$. Each segment has two end points, one on the left and one on the right, identified by the indices $\ell(j)$ and $r(j)$, respectively. The total amount of end points is denoted by N_p.

The discrete axial velocities are located at the center of the j-th segment and are denoted by u_j^n. Hence, the segments are the velocity control volumes and velocity is assumed to be constant in section j. To define a velocity direction for u_j^n we use the convention that the positive direction points from $\ell(j)$ to $r(j)$. The discrete pressure is denoted by p_i^n and is located at the end points of the segments. The set of segments that have the i-th pressure point in common is denoted by S_i, which means that if $j \in S_i$, then the i-th pressure point is an end point of the j-th segment. In this case we denote with $\wp(i,j)$ the neighbor of pressure point i on the common segment j. Since a staggered mesh is used, we also have to introduce the control volumes for pressure. For this purpose we will indicate with the i-th cell the pressure control volume element between the middle points of the j-th segment, for every $j \in S_i$. Finally, the discrete concentration of the substance C_i^n is located at the segment end points, like the pressure.