COMPUTATIONS OF AN UNSTEADY VISCOUS FLOW IN A THREE DIMENSIONAL SYSTEM OF DUCTS. PART I: FORMULATION OF THE MATHEMATICAL PROBLEM AND NUMERICAL METHOD

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Numerical modeling of an unsteady flow of a viscous incompressible fluid inside a branched pipe system is considered. The mathematical formulation is given with special emphasis on inlet/outlet conditions. The equivalent weak form of the initial-boundary value problem is presented. The numerical method based on solutions to particular Stokes problems is proposed and described in some details. Finally, some general remarks about the implementation issues within the framework of the spectral element discretization are made.

Key words: Navier-Stokes equations, defective boundary conditions, spectral element method

1. Introduction

Numerical simulations of time-dependent viscous flows inside complex duct systems have recently become increasingly interesting for Computational Fluid Dynamics (CFD) community. This interest seems also to be stimulated mostly by medical applications. During the last decade, significant progress in CFD techniques applied to biological flows has been achieved. Undoubtedly, highly accurate numerical simulation of various types of motion of bio-fluids is a serious challenge. Much effort has been done, for instance, to develop computational models of the human cardiovascular system. These attempts
are motivated mostly by medical needs – it is expected that future, reliable computational models would be useful in the optimization of various cardio-surgery procedures. The necessary condition for success in this respect is to develop computational models and techniques which give realistic results by taking into account all important features like pulsating character of motion, complicated geometry and compliance of branched vessels, and, at least, non-Newtonian rheology of blood.

In this work, we consider the problem of numerical simulation of an unsteady flow of a viscous incompressible fluid in a system of branched pipes. The focus is on the proper mathematical formulation of the problem with special emphasis on inlet/outlet conditions. These conditions are "defective" in a sense that they are based on averaged values of the pressure and/or the volume flux. The presented formulation is a generalization of the approach recently proposed by Formaggia et al. (2000). Some remarks on the numerical implementation of the spectral element method are made, leaving detailed description of the solver and the presentation of obtained results to the second part of the paper.

2. Mathematical formulation

We consider three-dimensional unsteady (pulsating) motion of a Newtonian fluid in a branched pipe system with certain number of inlet/outlet (I/O) sections (see Fig. 1).

The mathematical problem is to solve the Navier-Stokes and continuity equations

$$\partial_t v + \nabla v \cdot v = -\frac{1}{\rho} \nabla p + \nu \nabla^2 v \quad \nabla \cdot v = 0$$

subject to appropriate initial and boundary conditions. In the above, the symbols $v$, $p$, $\rho$ and $\nu$ denote velocity, pressure, mass density and kinematic viscosity, respectively. Since the mass density is a constant value, it is convenient to choose $\rho = 1$.

The boundary conditions are defined as follows. At the impermeable (material) part of the boundary $\Gamma$, the no-slip condition for the velocity is imposed, i.e. $v|_\Gamma = 0$. At the I/O sections $S_i$ ($i = 1, \ldots, N$), the following variants of the boundary conditions are considered:
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Fig. 1. The computational domain

- variant Volume Flux (VF)

\[
\Phi_i(v) \equiv \int_{S_i} v \cdot n \, ds = F_i(t) \quad i = 1, \ldots, N_{VF} \tag{2.2}
\]

\(F_i(t)\) – given,

- variant Average Pressure (AP)

\[
\frac{1}{|S_{N_{VF}+i}|} \int_{S_{N_{VF}+i}} p \, ds = P_i(t) \quad i = 1, \ldots, N_{AP} \tag{2.3}
\]

\(P_i(t)\) – given.

At each I/O section either VF or AP variant of the boundary conditions is imposed, and \(N_{VF} + N_{AP} = N\). Time variations of the volume fluxes or the averaged pressure are defined by the given functions \(F_i(t) \ (i = 1, \ldots, N_{VF})\) or \(P_i(t) \ (i = 1, \ldots, N_{AP})\), respectively.

The integral boundary conditions formulated above are of much interest because they are natural in most of practical situations. Indeed, the knowledge of temporal variations of either the section-averaged pressure or the volume flux can be usually assumed. In medical context, such data can be provided by measurements or by the lumped-parameter models of the cardiovascular system. On the other hand, the precise distributions of physical quantities (like pressure or velocity) at I/O sections are usually not available – they have to be evaluated in the solution process.
The question arises whether such "defective" boundary conditions can be incorporated in a mathematically consistent way into an initial-boundary problem to equations (2.1). Surprisingly enough, this problem has been given a rigorous mathematical treatment only recently. In their seminal paper, Heywood et al. (1996) showed that the boundary conditions formulated above can be accounted for in an appropriate variational formulation. Recently, Formaggia et al. (2000) have presented an improved variant of this approach. They used the Lagrange multipliers technique to VF-type boundary conditions that allowed for convenient simplification of the function spaces involved in the variational formulation. This approach is a theoretical basis of the current work. The novelty consists in admitting coexistence of the I/O sections with VF and AP boundary conditions, not considered in previous works.

The new VF/AP variational formulation of the problem goes as follows:

\textbf{Find}

- the velocity field \( v \in V = \{ v \in [H^1(\Omega)]^3 : v|_\Gamma = 0 \} \)
- the pressure field \( p \in Q = L^2(\Omega) \)
- the (time-dependent) Lagrange multiplies \( \lambda_i \in R, i = 1, ..., N_{VF} \)

\textbf{such that}

- for each \( v \in V : \)
  \[
  (\partial_t v + \nabla v \cdot v, v) + \nu (\nabla v, \nabla v) + \sum_{i=1}^{N_{VF}} \lambda_i \Phi_i(v) + \\
  + \sum_{i=1}^{N_{AP}} P_i(t) \Phi_{N_{VF}+i}(v) - (p, \nabla \cdot v) = 0
  \]

- for each \( q \in Q : (q, \nabla \cdot v) = 0 \)
- \( \Phi_i(v) = F_i(t), \ i = 1, ..., N_{VF} \)
- \( v|_{t=t_0} = v_0 \) (the initial condition).

Heywood et al. (1996) showed that the smooth solutions to this variational problem satisfy the following "classical" boundary conditions

\[
\begin{align*}
(p - \nu \partial_n v_n)|_{S_i} = \lambda_i & \quad i = 1, ..., N_{VF} \\
(p - \nu \partial_n v_n)|_{S_{N_{VF}+i}} = P_i(t) & \quad i = 1, ..., N_{AP} \\
\partial_n v_n|_{S_i} = 0 & \quad i = 1, ..., N
\end{align*}
\]

(2.4)
In the above, we use the notation $\partial_n v_n = (\nabla v \cdot n)$ and $\partial_n v_\tau = (\nabla v \cdot \tau)$, where $(\nabla v)_{ij} = \partial v_i/\partial x_j$.

It can be noticed that the corresponding boundary conditions do not have any direct physical interpretation. In particular, they are not formulated in terms of normal and tangent surface stress distributions. Indeed, the latter would involve only the symmetric part of the tensor $\nabla \cdot v$. The conditions (2.4) are sometimes referred to as "pseudo-traction" conditions.

tangent component of the surface stress vanishes identically and the distributions of the normal component are uniform at each inlet/outlet section. Moreover, the normal stress distributions at I/O sections of AP type are given directly as the functions $P_i(t)$ ($i = 1, ..., N_{AP}$), while at I/O sections of VF type these distributions are unknown and have to be determined so that the prescribed volume fluxes are achieved.

It should be emphasized that the boundary conditions implied by the variational formulation at the AP inlets/outlets are not, in general, equivalent to the condition for the averaged pressure (2.3). Instead, one has the following equality

$$\int_{S_i} [p - \nu(\nabla v \cdot n) \cdot n] \, dS = P_i(t)|_{S_i} \quad (2.5)$$

However, it can be shown that conditions (2.5) and (2.3) are equivalent if only the surface of the inlet/outlet section is flat, i.e. when it is obtained by a plane cut of the pipe. Indeed, in such a case, the following equality holds

$$\int_{S_i} (\nabla v \cdot n) \cdot n \, dS = 0 \quad (2.6)$$

In order to prove (2.6), we choose the coordinate system so that the first axis is perpendicular to the (flat) surface section $S_i$. Then the normal vector at each point of $S_i$ is defined as $n = [1, 0, 0]$, and the surface integral can be calculated as follows

$$\int_{S_i} (\nabla v \cdot n) \cdot n \, dS = \int_{S_i} \frac{\partial v_1}{\partial x_1} \, dS = - \int_{S_i} \left( \frac{\partial v_2}{\partial x_2} + \frac{\partial v_3}{\partial x_3} \right) \, dS =$$

$$= - \oint_{\partial S_i} (v_2 \eta_2 + v_3 \eta_3) \, dl = 0$$

In the above, we have used the continuity equation and the Green Theorem of the plane in order to transform the surface integral to the contour integral along $\partial S_i$. The unitary vector $\eta = [\eta_2, \eta_3]$ lies in the plane of the
pipe section $S_i$, and it is normal to the contour line $\partial S_i$. Since the velocity vanishes identically at the pipe wall, the contour integral is equal to zero.

Using (2.5) and (2.6), one finally concludes that

$$P_i(t) = \frac{1}{|S_i|} \int_{S_i} p \, dS$$

(2.7)

Note again that, for the above proof to work, one has to assume sufficient regularity of the solution to ensure the existence of the velocity derivatives and the pressure at the inlet/outlet surfaces (in the sense of traces).

In the end, the following comment should be made. If $N_{AP} > 0$, i.e. at least one I/O section has been equipped with AP boundary conditions then the pressure field is uniquely defined. On the other hand, one may like to impose I/O conditions of the VF type exclusively. If $N_{VF} = N$ then the functions $F_i(t), i = 1, ..., N$, must obey the following constraint $\sum_{i=1}^{N} F_i(t) \equiv 0$, implied by the volume (or mass) conservation. Moreover, the pressure field is defined up to an additive constant. It is actually more reasonable (and convenient) to set $N_{VF} = N - 1$ so that $N_{AP} = 1$, and choose $P_1(t) \equiv 0$. The volume will be conserved (within achievable numerical accuracy) due to the continuity equation, and pressure ambiguity will not occur.

3. Time integration schemes and semi-discrete forms of the variational problem

In order to solve an unsteady flow problem various time discretization schemes can be applied. The popular choice is the explicit/implicit approach, i.e. the use of an implicit integration scheme for the linear part and an explicit scheme for the nonlinear part of the Navier-Stokes equation. The advantage of this approach is that symmetric and positive definite linear problems have to be solved at each time step. In contrast, methods using the implicit (or semi-implicit) time discretization to the nonlinear terms lead to large nonlinear problems or, at least, to linear but usually not symmetric and indefinite problems which are much more difficult to solve efficiently. On the other hand, the explicit treatment of the nonlinear terms suffers from limitations due to stability requirements. This is why it is essential to use integration schemes with favorable stability properties. Such a family of stiff-stable multi-step schemes has been proposed by Karniadakis et al. (1991). Consider, for presentation
purposes, the model evolutionary equation with linear and nonlinear operators, denoted by $L$ and $N$, respectively

$$z'(t) = L(t, z(t)) + N(t, z(t)) \quad (3.1)$$

The mixed multi-step method is obtained by using the backward differentiation scheme (implicit) for the linear operator, and the linear extrapolation (explicit) scheme for the nonlinear operator. The general formula for the $K$-step method is

$$\frac{1}{\Delta t} \sum_{k=0}^{K} \beta_k z^{(n+1-k)} = L^{(n+1)} + \sum_{k=1}^{K} \alpha_k N^{(n+1-k)} \quad (3.2)$$

As usual, the upper index in the brackets indicates a time instant each term is evaluated at.

The values of the coefficients $\{\alpha_k, k = 1, ..., K\}$ and $\{\beta_k, k = 0, ..., K\}$ can be found by Karniadakis et al. (1991). As an example, we give the explicit formula for the 3rd order method

$$\frac{1}{\Delta t} \left( \frac{11}{6} z^{(n+1)} - 3 z^{(n)} + \frac{3}{2} z^{(n-1)} - \frac{1}{3} z^{(n-2)} \right) = L^{(n+1)} + 3 N^{(n)} - 3 N^{(n-1)} + N^{(n-2)} \quad (3.3)$$

More details on other schemes of this sort and their stability characteristics can be found in the cited paper.

When the multistep method, see (3.2), is used, variational problem (Problem 2.1) takes the following semi-discretized form

$$\frac{\beta_0}{\Delta t} (v^{(m+1)}, v) + \nu (\nabla v^{(m+1)}, \nabla v) - (p^{(m+1)}, \nabla \cdot v) + \sum_{i=1}^{N_{VF}} \Phi_i(v) \lambda_i^{(m+1)} =$$

$$= - \frac{1}{\Delta t} \sum_{k=1}^{K} \beta_k (v^{(m+1-k)}, v) - \frac{1}{\Delta t} \sum_{k=1}^{K} \alpha_k (\nabla v^{(m+1-k)} \cdot v^{(m+1-k)}, v) -$$

$$- \sum_{i=1}^{N_{AP}} P_i^{(m+1)} \Phi_{N_{VF}+i}(v) \quad (3.4)$$

$$(q, \nabla \cdot v^{(m+1)}) = 0 \quad \Phi_i(v^{(m+1)}) = F_i(t) \quad i = 1, ..., N_{VF}$$

A different mixed explicit/implicit integration scheme has been proposed by Maday et al. (1990). It consists in splitting the integration of nonlinear
(advective) and linear parts of the Navier-Stokes equation, i.e. these parts are treated separately. Formally, the method is based on the construction of the operator integration factor for the advective part. However, it can be shown that this operator does not need to be constructed explicitly.

In the sequel, we will provide short and informal derivation of the operator-integration-factor splitting (OIFS) method. The reader should refer to the original paper (Maday et al., 1990) for a more rigorous and detailed exposition.

Consider model equation (3.1) with the assumption that the nonlinear part is autonomous, i.e. it does not depend explicitly on time. Let \( u(t) \) be an arbitrary function satisfying the differential equation \( \frac{du(t)}{dt} = N(u(t)) \). Then, we assume the existence of the operator integration factor \( Q(\tau,t) \) such that

\[
Q(\tau,\tau) = \text{Id}
\]

and

\[
\frac{d}{dt} \left[ Q(\tau,t) z(t) \right] = 0
\]

(3.6)

Assuming the continuity of the nonlinear operator \( N \), and taking into account the initial condition \( u(\tilde{t}) = z(\tilde{t}) \), the following equality holds at \( t = \tilde{t} \)

\[
\frac{d}{dt} \left[ Q(\tau,t) z(t) \right] \bigg|_{t=\tilde{t}} = Q(\tau,\tilde{t}) L(z(\tilde{t}))
\]

(3.8)

The two remaining components in the right-hand side of equation (3.7) vanish identically at \( t = \tilde{t} \). Moreover, it is reasonable to neglect these terms also for \( t \) slightly larger than \( \tilde{t} \) as they depend only on difference between the values of the functions \( u \) and \( z \). In other words, we assume that simplified equation (3.8) is approximately valid over the short time interval \( (\tilde{t} \equiv t_n, \tilde{t} + \Delta t) \).
\[ \tau = \tilde{t} + \Delta t \equiv t_{n+1}. \] Now, we integrate this equation numerically, performing one step with the implicit method based of the backward differentiation of the \( K \)th order

\[
\frac{1}{\Delta t} \sum_{k=0}^{K} \beta_k Q(t_{n+1}, t_{n+1-k}) z(t_{n+1-k}) = Q(t_{n+1}, t_{n+1}) L(z(t_{n+1})) \quad (3.9)
\]

With the use of equality (3.6), one can get rid of any explicit reference to the operator \( Q \) in (3.9) and finally obtain the following linear equation

\[
\frac{\beta_0}{\Delta t} z(t_{n+1}) - L(z(t_{n+1})) = -\frac{1}{\Delta t} \sum_{k=1}^{K} \beta_k u_k(t_{n+1}) \quad (3.10)
\]

In the above, the functions \( u_k \) \( (k = 1, \ldots, K) \) are the solutions to the following initial value problems

\[
\frac{d}{dt} u_k(t) = N(u_k(t)) \quad t \in (t_{n+1-k}, t_{n+1}) \quad (3.11)
\]

\[
u_k(t_{n+1-k}) = z(t_{n+1-k})
\]

Initial value problems (3.11) are solved using a suitable explicit integration scheme. In hydrodynamic applications, where the nonlinearity is due to the advective part of the fluid acceleration, the 4th order explicit Runge-Kutta method is preferred. Usually, only a few steps are done to march over the time interval \( \Delta t \). Note that the number of the evaluation of the operator \( N \) becomes quite large when the number of sub-steps as well as the order of the backward differentiation get larger. If, for instance, \( K = 3 \) and five RK4 sub-steps are used per each time interval \( \Delta t \) then the number of the evaluations of the operator \( N \) is 120.

In the context of the flow problem considered in this study, the OIFS method described above can be written as follows

\[
\frac{\beta_0}{\Delta t} (v^{(m+1)}, v) + \nu (\nabla v^{(m+1)}, \nabla v) - (p^{(m+1)}, \nabla \cdot v) + \sum_{i=1}^{N_{VF}} \Phi_i(v) \lambda_i^{(m+1)} =
\]

\[
= -\frac{1}{\Delta t} \sum_{k=1}^{K} \beta_k (\hat{v}_k^{(m+1)}, v) - \sum_{i=1}^{N_{AP}} P_i^{(m+1)} \Phi_{N_{VF}+i}(v) \quad (3.12)
\]

\[
(q, \nabla \cdot v^{(m+1)}) = 0 \quad \Phi_i(v^{(m+1)}) = F_i(t) \quad i = 1, \ldots, N_{VF}
\]

In the above, the vector fields \( \hat{v}_k^{(m+1)} \) are defined as \( \hat{v}_k^{(m+1)} \equiv \hat{v}_k(t_{m+1}) \) where \( \hat{v}_k, k = 1, \ldots, K \), are obtained as the approximate solutions to the
following initial value problems
\[
\frac{\partial}{\partial t} \hat{v}_k = -\nabla \hat{v}_k \cdot \hat{v}_k \quad t \in (t_{m+1-k}, t_{m+1})
\]
(3.13)

\[
\hat{v}_k(t_{m+1-k}) = v(t_{m+1-k}) \equiv v^{(m+1-k)}
\]

Couzy (1995) tested systematically the OIFS method and compared then the multi-step methods proposed by Karniadakis et al. (1991). The OIFS schemes proved to be superior in terms of stability properties (except for cases of low Reynolds numbers where the multi-step methods become unconditionally stable). On the other hand, the multi-step methods are free from the splitting error and usually provide better accuracy. Superior stability properties of the OIFS schemes make them more suitable for computations of laminar flows with larger Reynolds numbers, blood flows in large vessels being an example.

4. Space discretization

In order to obtain a tractable algebraic problem, one has to set up a space discretization. The first step of this procedure is to define appropriate finite dimensional function spaces. These spaces are spanned by a finite number of basic functions. The velocity is approximated as a linear combination of the $3N_V$ basic vector fields from the function space $V$ (see the Section 2) defined as

\[
v_1 = [w_1, 0, 0] \quad v_2 = [w_2, 0, 0] \quad \cdots \quad v_{N_V} = [w_{N_V}, 0, 0]
\]

\[
v_{N_V+1} = [0, w_1, 0] \quad v_{N_V+2} = [0, w_2, 0] \quad \cdots \quad v_{2N_V} = [0, w_{N_V}, 0]
\]

\[
v_{2N_V+1} = [0, 0, w_1] \quad v_{2N_V+2} = [0, 0, w_2] \quad \cdots \quad v_{3N_V} = [0, 0, w_{N_V}]
\]
(4.1)

Analogously, the pressure field will be approximated within the finite dimensional subspace of $Q$ spanned by the basic (scalar) functions $q_1, q_2, \ldots, q_{N_P}$. With the use of the discrete function spaces defined above, the unknown velocity and pressure field can be expressed as

\[
v^{(m+1)} = \sum_{j=1}^{N_V} (u_1^{(m+1)})_j v_j + \sum_{j=1}^{N_V} (u_2^{(m+1)})_j v_{N_V+j} + \sum_{j=1}^{N_V} (u_3^{(m+1)})_j v_{2N_V+j}
\]

\[
p^{(m+1)} = \sum_{j=1}^{N_P} (\pi^{(m+1)})_j q_j
\]
(4.2)
Let us define the following indexed structures:

\[(M_V)_{ij} = (w_i, w_j) \equiv \int_{\Omega} w_i w_j \, dx \quad i, j = 1, ..., N_V\]

\[(K_V)_{ij} = (\nabla w_i, \nabla w_j) \equiv \int_{\Omega} \nabla w_i \cdot \nabla w_j \, dx \quad i, j = 1, ..., N_V\]

\[A = \frac{\beta_0}{\Delta t} M_V + \nu K_V\]  \hspace{1cm} (4.3)

\[(\Lambda_1^F)_{ij} = \Phi_i(v_j) \quad i = 1, ..., N_{VF}, \quad j = 1, ..., N_V\]

\[(\Lambda_2^F)_{ij} = \Phi_{N_F+i}(v_j) \quad i = 1, ..., N_{AP}, \quad j = 1, ..., N_V\]

\[(\Lambda_3^F)_{ij} = \Phi_{N_F+i}(v_j) \quad i = 1, ..., N_{VF}, \quad j = N_V + 1, ..., 2N_V\]

\[(\Lambda_3^F)_{ij} = \Phi_{N_F+i}(v_j) \quad i = 1, ..., N_{VF}, \quad j = 2N_V + 1, ..., 3N_V\]

\[(\Lambda_3^F)_{ij} = \Phi_{N_F+i}(v_j) \quad i = 1, ..., N_{AP}, \quad j = 2N_V + 1, ..., 3N_V\]

\[(D_{\alpha})_{ij} = -(q_i, \partial_{X_\alpha} w_j) \quad i = 1, ..., N_Q, \quad j = 1, ..., N_V, \quad \alpha = 1, 2, 3\]

\[(P)_{i} = P_i \quad i = 1, ..., N_{AP}\]

\[(F)_{i} = F_i \quad i = 1, ..., N_{VF}\]

Now, the algebraic problem to be solved at each time step of the numerical simulation can be written in the form of

\[
\begin{bmatrix}
A & 0 & 0 & (D_1)^\top & (\Lambda_1^F)^\top \\
0 & A & 0 & (D_2)^\top & (\Lambda_2^F)^\top \\
0 & 0 & A & (D_3)^\top & (\Lambda_3^F)^\top \\
D_1 & D_2 & D_3 & 0 & 0 \\
\Lambda_1^F & \Lambda_2^F & \Lambda_3^F & 0 & 0
\end{bmatrix}
\begin{bmatrix}
u_1 \\
u_2 \\
u_3 \\
\pi \\
\lambda
\end{bmatrix}^{(m+1)} =
\begin{bmatrix}
(r_1 - (\Lambda_1^F)^\top P)^{(m+1)} \\
(r_2 - (\Lambda_2^F)^\top P) \\
(r_3 - (\Lambda_3^F)^\top P) \\
0 \\
F
\end{bmatrix}
\hspace{1cm} (4.4)
\]

The detailed structure of the right-hand side vector depends on the time discretization scheme used. In the \(K\)th order multi-step method, the vectors \(r_{(*)}^{(m+1)}\) are defined as

\[
\begin{bmatrix}
n(r_{(*)})^{(m+1)}
\end{bmatrix}_i = -\frac{1}{\Delta t} \sum_{k=1}^{K} \beta_k \left( (v^{(m+1-k)}), w_i \right) +
\]

\[
- \sum_{k=1}^{K} \alpha_k \left( (\nabla v^{(m+1-k)} \cdot v^{(m+1-k)}), w_i \right) \quad i = 1, ..., N_V
\]  \hspace{1cm} (4.5)
while in the case of the OIFS scheme,

\[
\left( r^{(m+1)}_{(*)} \right)_i = -\frac{1}{\Delta t} \sum_{k=1}^{K} \beta_k \left( (\hat{v}^{(m+1)}_k)_{(*)}, w_i \right) \quad i = 1, ..., N_V
\]

(4.6)

where \( \hat{v}^{(m+1)}_k \) have been defined by (3.13).

In formulas (4.5) and (4.6), the subscript \((*)\) indicates the Cartesian component, i.e. it stands for either 1, 2 or 3.

5. Construction of the solution at each time step

Assuming a fixed time step in the integration scheme, we propose the following method of dealing with algebraic problem (4.4).

Consider the following linear systems of equations \((k = 1, ..., N_{VF} + N_{AP})\)

\[
\begin{bmatrix}
A & 0 & 0 & (D_1)^T \\
0 & A & 0 & (D_2)^T \\
0 & 0 & A & (D_3)^T \\
D_1 & D_2 & D_3 & 0
\end{bmatrix}
\begin{bmatrix}
\bar{u}^{[k]}_1 \\
\bar{u}^{[k]}_2 \\
\bar{u}^{[k]}_3 \\
\pi^{[k]}
\end{bmatrix}
= 
\begin{bmatrix}
-(\Lambda^F_1)^T \lambda^{[k]}_1 \\
-(\Lambda^F_2)^T \lambda^{[k]}_2 \\
-(\Lambda^F_3)^T \lambda^{[k]}_3 \\
0
\end{bmatrix}
\]

(5.1)

where

\[
\lambda^{[k]}_j = \begin{cases} 
0 & \text{if } j \neq k \\
1 & \text{if } j = k 
\end{cases}
\]

The solutions to the above systems will be referred to as the particular Stokes solutions. For each such solution, we introduce a vector containing values of the volume flux through all inlets/outlets

\[
f^{[k]} = \begin{bmatrix}
\Lambda^F_1 \\
\Lambda^P_1 \\
\Lambda^F_2 \\
\Lambda^P_2 \\
\Lambda^F_3 \\
\Lambda^P_3
\end{bmatrix}
\begin{bmatrix}
\bar{u}^{[k]}_1 \\
\bar{u}^{[k]}_2 \\
\bar{u}^{[k]}_3 \\
\pi^{[k]}
\end{bmatrix}
\]

\[
k = 1, ..., N_{VF} + N_{AP}
\]

(5.2)

If the geometry of the flow domain and the time step are fixed, all particular solutions can be computed once and forever.

Next, we define an additional problem as follows

\[
\begin{bmatrix}
A & 0 & 0 & (D_1)^T \\
0 & A & 0 & (D_2)^T \\
0 & 0 & A & (D_3)^T \\
D_1 & D_2 & D_3 & 0
\end{bmatrix}
\begin{bmatrix}
\bar{u}^{[0]}_1 \\
\bar{u}^{[0]}_2 \\
\bar{u}^{[0]}_3 \\
\pi^{[0]}
\end{bmatrix}
= 
\begin{bmatrix}
r_1 \\
r_2 \\
r_3 \\
0
\end{bmatrix}
\]

(5.3)
Again, the vector of the volume fluxes is computed as

$$f^{\{0\}} = \begin{bmatrix} \Lambda^F_1 \\ \Lambda^P_1 \end{bmatrix} u_1^{\{0\}} + \begin{bmatrix} \Lambda^F_2 \\ \Lambda^P_2 \end{bmatrix} u_2^{\{0\}} + \begin{bmatrix} \Lambda^F_3 \\ \Lambda^P_3 \end{bmatrix} u_3^{\{0\}} (5.4)$$

Note that, in contrast to systems (5.1), the set of equations (5.3) has to be solved at each time step of the flow simulation.

The solution to the full Stokes problem (4.4) can be now expressed as the following superposition

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \pi \end{bmatrix} = \begin{bmatrix} u_1^{\{0\}} \\ u_2^{\{0\}} \\ u_3^{\{0\}} \\ \pi^{\{0\}} \end{bmatrix} + \sum_{k=1}^{N_{VF}} \lambda_k \begin{bmatrix} u_1^{\{k\}} \\ u_2^{\{k\}} \\ u_3^{\{k\}} \\ \pi^{\{k\}} \end{bmatrix} + \sum_{k=1}^{N_{AP}} P_k \begin{bmatrix} u_1^{\{N_{VF}+k\}} \\ u_2^{\{N_{VF}+k\}} \\ u_3^{\{N_{VF}+k\}} \\ \pi^{\{N_{VF}+k\}} \end{bmatrix} (5.5)$$

The last term in the right-hand side of expression (5.5) contains the given values of the averaged pressures $P_k$ ($k = 1, ..., N_{AP}$). The multipliers $\lambda_k$, $k = 1, ..., N_{VF}$, are evaluated at the given time step from the following linear system

$$T_F \lambda = F - f^{\{0\}}_{VF} - T_P P \quad (5.6)$$

where

$$T_F = \begin{bmatrix} f^{\{1\}}_{1} & \cdots & f^{\{N_{VF}\}}_{1} \\ \vdots & \ddots & \vdots \\ f^{\{1\}}_{N_{VF}} & \cdots & f^{\{N_{VF}\}}_{N_{VF}} \end{bmatrix} \quad T_P = \begin{bmatrix} f^{\{N_{VF}+1\}}_{1} & \cdots & f^{\{N_{VF}+N_{AP}\}}_{1} \\ \vdots & \ddots & \vdots \\ f^{\{N_{VF}+1\}}_{N_{VF}} & \cdots & f^{\{N_{VF}+N_{AP}\}}_{N_{VF}} \end{bmatrix} \quad (5.7)$$

and $f^{\{0\}}_{VF} \equiv f^{\{0\}} (1 : N_{VF})$. Note that the matrix $T_F$ is nonsingular as long as $N_{VF} < N$.

Summarizing, at each time step we have to solve Stokes problem (5.3) in order to get $\{u_1^{\{0\}}, u_2^{\{0\}}, u_3^{\{0\}}, \pi^{\{0\}}\}$, and then solve small linear system (5.6) to evaluate the Lagrange multipliers.

In the end, we briefly consider the particular case. Assume that $N_{AP} = N$, which means that all inlet/outlet conditions are formulated in terms of the average pressure. In such a case, the volume flux through each I/O section follows uniquely from prescribed inlet/outlet pressures driving the flow, and the Lagrange multipliers do not appear in the mathematical formulation. The method based on the superposition described above still works, but this time
the solution can be obtained directly by solving the following Stokes problem

\[
\begin{pmatrix}
A & 0 & 0 & (D_1)^T \\
0 & A & 0 & (D_2)^T \\
0 & 0 & A & (D_3)^T \\
D_1 & D_2 & D_3 & 0
\end{pmatrix}
\begin{pmatrix}
u_1 \\
u_2 \\
u_3 \\
\pi
\end{pmatrix}
= \begin{pmatrix}
r_1 - (\Lambda_1 P)^T P \\
r_2 - (\Lambda_2 P)^T P \\
r_3 - (\Lambda_3 P)^T P \\
0
\end{pmatrix}
\]  

(5.8)

In the above, the vector \( P \) is defined as \( P = [P_1^{(m+1)}, P_2^{(m+1)}, ..., P_N^{(m+1)}] \), i.e. it contains the values of the assumed averaged pressure at all inlets/outlets, at the time instant \( t = t_{m+1} \).

If all inlet/outlets conditions are formulated exclusively in terms of the volume fluxes one has to proceed as explained at the end of Section 2.

### 6. Solution to the Stokes problem

In this Section, the solution method for the algebraic Stokes problem

\[
A\alpha + D_\alpha^T = b_\alpha \quad \alpha = 1, 2, 3
\]

\[
\sum_{\alpha=1}^{3} D_\alpha u_\alpha = 0
\]

is considered. First, let us remind that system of equations (6.1) can be solved using the following triple-step procedure (Schur-complement method, see Formaggia et al., 2000)

\[
\begin{align}
(1) & \quad A\tilde{u}_\alpha = b_\alpha \quad \alpha = 1, 2, 3 \\
(2) & \quad \pi \sum_{\alpha=1}^{3} D_\alpha A^{-1} D_\alpha^T = \sum_{\alpha=1}^{3} D_\alpha \tilde{u}_\alpha \\
(3) & \quad A u_\alpha = -D_\alpha^T \pi + b_\alpha \quad \alpha = 1, 2, 3
\end{align}
\]

At each step in (6.2), a symmetric and positive-definite (SPD) algebraic problem is to be solved. In most practical situations, the preconditioned conjugate gradient method (PCCGM) would be a solver of the first choice. The efficient preconditioning of the second (pressure) step is crucial. A number of sophisticated preconditioners have been proposed during the last decade, see, for instance, Maday et al. (1993) or Couzy and Deville (1994) and references
therein. The linear systems with the Helmholtz matrix $A$ have to be solved during the first and third step. Since the Helmholtz matrix $A$ is usually strongly diagonally dominant, the numerical solution can be efficiently computed using PCGM even with simple preconditioners (like a diagonal one).

In numerical simulations of nonstationary flows with higher Reynolds numbers and small time steps, the computational time of steps (1) and (3) is almost negligible with respect to step (2). In order to reduce computational cost of the pressure evaluation, various approximate inversion methods for the matrix $A$ have been proposed. We will focus on the method proposed recently by Quarteroni et al. (1999). In order to avoid expensive inversion of the matrix

$$A = \frac{\beta_0}{\Delta t} M_V + \nu K_V$$

the following approximation of $A^{-1}$ based on the truncated Neumann series can be used

$$A^{-1} = \frac{\Delta t}{\beta_0} \left( I - \frac{\nu \Delta t}{\beta_0} M_V^{-1} K_V \right)^{-1} M_V^{-1} \approx$$

$$\approx \frac{\Delta t}{\beta_0} M_V^{-1} - \nu \left( \frac{\Delta t}{\beta_0} \right)^2 M_V^{-1} K_V M_V^{-1} + \nu^2 \left( \frac{\Delta t}{\beta_0} \right)^3 M_V^{-1} (K_V M_V^{-1})^2 \equiv H \quad (6.3)$$

Approximation (6.3) is computationally efficient providing that the velocity mass matrix is easily invertible. In particular, pseudo-spectral (or spectral collocation) discretization leads to purely diagonal mass matrices for both velocity and pressure. The matrix $H$ is always positive definite as long as the number of terms in the truncated Neumann series is odd.

Another useful modification of original algorithm (6.2) is its reformulation into an incremental variant. In the course of numerical simulation of an unsteady flow, the solver will usually carry out tiny time steps, and the instantaneous pressure distributions obtained in two subsequent steps will not be much different. In other words, it is reasonable to expect that the solution in the current time step will serve as a good starting point for the iterations in the next time step. Therefore, we assume that the pressure vector is expressed as

$$\pi = \pi_* + \pi'$$

where $\pi_*$ denotes an available approximation of the unknown vector $\pi$ (the pressure vector from the previous time step is a natural candidate), while $\pi'$ is the correction to be evaluated. Following these lines, we introduce also the velocity corrections $u'_1$, $u'_2$ and $u'_3$ defined by the following expressions

$$u_\alpha = \tilde{u}_\alpha + u'_\alpha \quad \alpha = 1, 2, 3$$

$$\quad (6.5)$$
Now, the incremental version of the algorithm using approximation (6.3) can be summarized as follows

\begin{align*}
(1) \quad & A\tilde{u}_\alpha = b_\alpha - D_\alpha^T \pi_* \quad \alpha = 1, 2, 3 \\
(2) \quad & \pi' \sum_{\alpha=1}^{3} D_\alpha HD_\alpha^T = \sum_{\alpha=1}^{3} D_\alpha \tilde{u}_\alpha \quad \text{(6.6)} \\
(3) \quad & A u'_\alpha = -D_\alpha^T \pi' \quad \alpha = 1, 2, 3 
\end{align*}

Having the corrections of the velocity components and pressure field computed, formulas (6.4) and (6.5) are used to obtain the complete solution.

It is worth mentioning that approximation (6.4) can be interpreted in terms of artificial compressibility. Indeed, the continuity equation corresponding to the approximated inverse is no longer homogeneous; instead, the following form can be derived

\[ \sum_{\alpha=1}^{3} D_\alpha u_\alpha = \pi \sum_{\alpha=1}^{3} D_\alpha (H - A^{-1})D_\alpha^T \quad \text{(6.7)} \]

It can be seen that, accordingly to (6.3), the error of incompressibility incurred by the approximated inverse is \( \sim O(\Delta t^3) \).

It spite of the apparently complicated structure of inverse formulae (6.3), the product \( Hr \) (here \( r \) denotes an arbitrary vector) can be computed in a simple way, namely

\[ w^{(1)} = \frac{\Delta t}{\beta_0} M^{-1} r \quad \text{(6.8)} \]

for \( j = 1, \ldots, m - 1 \) repeat

\[ w^{(j+1)} = \frac{\Delta t}{\beta_0} M^{-1} (-\nu KW^{(j)} + r) \quad \text{(6.9)} \]

In the above, the integer \( m \) denotes the order of the approximation or, equivalently, the number of terms of the truncated Neumann expansion. As it has already been mentioned, it is recommended to choose \( m \) as an odd number, otherwise the matrix \( H \) may not be positive definite. Note that for formula (6.3) we have \( m = 3 \).

7. General remarks on numerical implementation

In order to numerically simulate complicated flows in the cardiovascular system, a numerical method should provide a high level of spatial resolution.
It is also necessary for the method to be capable of accurate prediction of flow characteristics which are calculated from the velocity field by means of differentiation (e.g. shear stress). Therefore, the spatial representation of the velocity and pressure fields should be sufficiently regular. The spectral element discretization seems to be an appropriate choice as it combines geometric flexibility with the ability to provide sufficient spatial accuracy with a reasonable number of unknowns. Within this approach, a wide spectrum of particular techniques exists.

Here we briefly characterize an approach used in the current work. The method of our choice is the "classical" spectral collocation (or pseudo-spectral) method using the hexahedral Lagrangian elements. It means that the local basic functions are the Lagrangian interpolating polynomials defined for the Jacobi/Legendre grid nodes inside each element. The differentiation with respect to space variables is carried out with the use of (pseudo-spectral) differentiating matrices. The volume integrals are evaluated by means of the Gauss-Legendre quadratures defined with the use of the same sets of the nodes as the basic functions. The detailed description of this "numerical technology" can be found in the monographs by Canuto et al. (1988) and Karniadakis and Sherwin (1999).

As it has already been mentioned, the fundamental blocks of the numerical method are the Helmholtz problem (if approximated inverse (6.6) is used, this problem is solved exactly six times at each time step) and pressure problem (6.5). Both problems lead, after the spatial discretization, to the symmetric and positive definite linear algebraic systems. The pressure problem is much more difficult to solve since it requires an appropriate preconditioning method. A large amount of theoretical work in the last fifteen years has been devoted to the development of efficient and robust preconditioning techniques for algebraic problems arising from hydrodynamic equations. One of the essential conclusions is that the matrix

\[
P^{-1} = \nu M_P^{-1} + \frac{\beta_0}{\Delta t} \sum_{\alpha=1}^{3} (D_{\alpha} M^{-1}_V D_{\alpha}^\top)^{-1}
\]

is spectrally close to the inverse of the matrix of the pressure problem (step (2) in (6.2)). In the above, \( M_P \) denotes the pressure mass matrix. The use of this preconditioner is not an easy task, though. The matrix inside the brackets

\[
E = \sum_{\alpha=1}^{3} D_{\alpha} M^{-1}_V D_{\alpha}^\top
\]

is itself very poorly conditioned (see Maday et al, 1993). Thus, the linear system with the matrix \( E \) cannot be solved efficiently without another low-level
preconditioner. In the case of hexahedral grids, the block preconditioner based on the local Fast Diagonalization Method (FDM) proved to be effective, as described by Couzy (1995), Couzy and Deville (1994). The complete description of this technique and its implementation in the current work will be given in the second part of the paper.

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References


**Wyznaczanie nieustalonych przepływów cieczy lepkiej w trójwymiarowym układzie przewodów. Część I: Sformułowanie problemu i opis metody numerycznej**

Streszczenie

W pracy rozważono problem numerycznego wyznaczania nieustalonego przepływu cieczy lepkiej w układzie trójwymiarowych przewodów. Podano sformułowanie wariacyjne zagadnienia uwzględniające uogólnione warunki brzegowe na wlotach/wylotach do obszaru ruchu. Opisano metodę obliczeniową, opartą na zastosowaniu wskaźników Lagrange’a i superpozycji szczególnych problemów Stokesa w każdym kroku czasowym.

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