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Large eddy simulation of powered Fontan hemodynamics

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ABSTRACT

Children born with univentricular heart disease typically must undergo three open heart surgeries within the first 2–3 years of life to eventually establish the Fontan circulation. In that case the single working ventricle pumps oxygenated blood to the body and blood returns to the lungs flowing passively through the Total Cavopulmonary Connection (TCPC) rather than being actively pumped by a subpulmonary ventricle. The TCPC is a direct surgical connection between the superior and inferior vena cava and the left and right pulmonary arteries. We have postulated that a mechanical pump inserted into this circulation providing a 3–5 mmHg pressure augmentation will reestablish bi-ventricular physiology serving as a bridge-to-recovery, bridge-to-transplant or destination therapy as a "biventricular Fontan" circulation. The Viscous Impeller Pump (VIP) has been proposed by our group as such an assist device. It is situated in the center of the 4-way TCPC intersection and spins pulling blood from the vena cavae and pushing it into the pulmonary arteries. We hypothesized that Large Eddy Simulation (LES) using high-order numerical methods are needed to capture unsteady powered and unpowered Fontan hemodynamics. Inclusion of a mechanical pump into the CFD further complicates matters due to the need to account for rotating machinery. In this study, we focus on predictions from an in-house high-order LES code (WenoHemo^{TM}) for unpowered and VIP-powered idealized TCPC hemodynamics with quantitative comparisons to Stereoscopic Particle Imaging Velocimetry (SPIV) measurements. Results are presented for both instantaneous flow structures and statistical data. Simulations show good qualitative and quantitative agreement with measured data.

1. Introduction

Compared to normal circulation, children born with single ventricle heart disease typically undergo a series of three staged open heart surgeries within the first 2–3 years of life to eventually live with a Fontan circulation (Gewillig, 2005). The anatomy of the Fontan circulation involves a direct connection between the Superior and Inferior Vena Cavae (SVC and IVC) and the Right and Left Pulmonary Arteries (RPA and LPA) forming the Total Cavopulmonary Connection or TCPC. Effectively, these patients have a single working ventricle which pumps oxygenated blood to the body and deoxygenated blood passively flows through the TCPC to the lungs in series, but without a subpulmonary power source. It is an inherently inefficient circulation which is associated with elevated systemic venous pressures and reduced ventricular filling (Deleval, 1998). The TCPC hemodynamics effectively involve two confined impinging jets and complex unsteady chaotic vortical flow patterns resulting in undesirable pressure loss and irregular streaming. For more than the past decade researchers have focused on reducing pressure losses at the TCPC junction by passive geometric means such as introducing offset (Migliavacca et al., 2003), or splitting the SVC and/or IVC (Soerensen et al., 2007; Marsden et al., 2009). Those solutions prevent the two jets coming from the IVC and SVC from colliding. By doing so, the competition between the two jets is avoided, and so are the strong pressure losses. In contrast, our group has focused on a cavopulmonary assist device, which consists in inserting a mechanical pump into the Fontan circulation to provide the estimated 3–5 mmHg needed to reestablish normal biventricular pressure levels as a means to bridge-to-recovery or bridge-to-transplant (Rodefeld et al., 2003). Previous designs have been proposed, from axial blood pumps placed in the vena cavae (Rodefeld et al., 2003) to a folding propeller design (Throckmorton et al., 2007). Our current design has evolved substantially from prior device concepts, is based on the von Karman viscous pump principle and involves spinning a double-sided cone featuring 6 mild vanes at the center of the TCPC junction (Rodefeld et al., 2010). The pump design is motivated by the desire for a percutaneous expandable rotary blood pump. This pump could be used to reduce the number of surgeries required for the survival of the infants from three to two or even one. In addition, this would minimize the Fontan-related disease caused by the current staged procedures while older. This pump would also be used in older patients showing signs of heart failure. Placing a right-sided power source in the univentricular Fontan circulation will

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restore conditions closer to a normal two-ventricle circulation. This will ease the symptoms of Fontan failure and allow the physician to take care of the patient as a "biventricular Fontan". Preliminary performance, biocomptability and CFD studies of a rigid prototype-have demonstrated the feasibility of the Viscous Impeller Pump (VIP) (Kennington et al., 2011; Giridharan et al., in press).

Computational fluid dynamics (CFD) of pathological and medical device hemodynamics has become very popular over the past decade due to the widespread availability of medical images, associated processing software, and open-source and commercial CFD packages. Many of these studies assume laminar flow or use Reynolds Averaged Navier–Stokes (RANS) based turbulence models for predictions. This is potentially a problem when dealing with pathological and medical device hemodynamics due to the flow regime being transitional or low Reynolds number turbulence, and featuring flow curvature and rotation. Traditional RANS-based turbulence models are known to have accuracy issues in dealing with these flow features. These issues were recently brought out in paper reporting on an FDA-approved computational and experimental study of an idealized medical device (Stewart et al., 2012). In addition, blood damage prediction models typically require accurate predictions of instantaneous wall shear stress and flow residence time, and this information is typically not available in a RANS simulation. Other simulations of Fontan circulation involved the use of low order finite element methods allowing an easier coupling between fluid and solid domains (Marsden et al., 2009).

In this study, the focus is on Large Eddy Simulation (LES) and its potential to predict pathological and medical device hemodynamics. In LES the large-scale unsteady three-dimensional flow features are numerically resolved and the effect of the unresolved small-scale eddies on the large-scales is modeled using a Subgrid-Scale (SGS) model (Pope, 2000). While it is debatable, there is a general consensus in the literature that LES calls for the use of a high-order numerical method to accurately capture the still relatively wide-range of large eddy length scales. The use of high-order numerical methods often makes application to complex geometries, especially those involving patient-specific geometries and rotating machinery, difficult. Also, accurate SGS models that can handle transitional flows are still a challenge. Furthermore, validation of LES predictions through quantitative comparisons to measured velocity profiles, and not just more global measures like pressure drop or pump performance, is critical.

Our approach is based on the use of a finite-difference method using a structured Cartesian grid combined with a version of the immersed boundary method for handling complex geometries and rotating machinery. In the next section, the computational method is described in detail. This is followed by a brief description of the experimental method used to obtain the measured data for validation. More details on this experiments and a full description of the measurements appear in a separate publication (Kerlo et al., 2011). Following, LES results for unpowered and powered Fontan hemodynamics are presented with comparisons to measured data. A summary concludes the paper.

2. Methods

2.1. LES equations

The filtered incompressible Navier–Stokes equations solved in our in-house code (WenoHemo^{TM}) are

$$\frac{\partial \overline{u}_i}{\partial t}+\overline{u}_j\frac{\partial \overline{u}_i}{\partial x_j}=-\frac{\partial \overline{p}}{\partial x_i}+\frac{1}{Re}\frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_j}-\frac{\partial \tau_{ij}}{\partial x_j} \tag{1}$$

$$\frac{\partial \overline{u}_i}{\partial x_i}=0 \tag{2}$$

where $\overline{u}_i$ is the ith component of the spatially filtered velocity vector, $\overline{p}$ is the spatially filtered pressure, x_i is the ith component of the spatial domain and τ_{ij} is the sub-grid stress tensor which arises from the filtering of the equations, and is defined as

$$\tau_{ij}=\overline{u_i u_j}-\overline{u}_i\overline{u}_j-\tfrac{2}{3}(\overline{u_j u_j}-\overline{u}_j\overline{u}_j)\delta_{ij} \tag{3}$$

All the parameters (velocities, spatial variables, ...) are dimensionless. In the case of the TCPC simulations, the velocity is non dimensionalized using the inlet velocity U_{inlet} and the physical dimensions are non-dimensionalized using the inlet diameter D.

The Vreman SGS turbulence model is employed in this study. The SGS stress tensor τ_{ij} is related to the filtered strain rate tensor S_{ij} using an eddy viscosity ν_T, where

$$\tau_{ij}=-2\nu_T S_{ij} \tag{4}$$

$$\begin{cases} \nu_T = C \times M(\overrightarrow{u}) \\ S_{ij}=\dfrac{1}{2}\left(\dfrac{\partial \overline{u}_i}{\partial x_j}+\dfrac{\partial \overline{u}_j}{\partial x_i}\right) \end{cases} \tag{5}$$

The model for the kernel $M(\overrightarrow{u})$, originally proposed by Vreman (2004) and tested in the present code by Shetty et al. (2010), is robust and easy to implement. The kernel is a function of the components of the velocity gradient tensor. The constant C arises from the Vreman model and its value can vary as a function of the case studied. In our case, the value of the constant used is 0.07. More details on the eddy viscosity formula are provided in the two papers cited above (Vreman, 2004; Shetty et al., 2010). Due to the form of the model kernel, the eddy viscosity goes to zero in laminar regions, as well as in near wall regions. These are important features of a SGS model for transitional wall-bounded flows such as those studied herein.

2.2. Numerical methods

In order to solve Eqs. (1) and (2), a predictor/corrector scheme is used. During the first stage, a predicted value of the velocity field u^* is obtained by solving Eq. (1) without the pressure term. The pressure field is then obtained by solving the following Poisson equation:

$$\frac{\partial^2 \overline{p}}{\partial x_i \partial x_i}=\frac{1}{\Delta t}\left(\frac{\partial \overline{u}_i^*}{\partial x_i}\right) \tag{6}$$

The velocity field is finally corrected to obtain $\overline{u}_i^{n+1}$, which now respects the continuity equation.

$$\overline{u}_i^{n+1}=\overline{u}_i^*-\Delta t\frac{\partial \overline{p}}{\partial x_i} \tag{7}$$

The time integration is performed using a third order accurate backward difference scheme (Shetty et al., 2011).

The convective terms in Eq. (1) are discretized using a fifth-order accurate Weighted Essentially Non-Oscillatory (WENO) scheme. The WENO scheme uses adaptive stencils to balance the desire for high-order accuracy with a non-oscillatory solution near discontinuities. This scheme uses upwinding based on the sign of the velocity multiplying the spatial derivative and chooses the smoothest stencil by avoiding the discontinuities in the interpolation process. The detailed of the scheme can be found in Zhang's paper (Zhang and Jackson, 2009). The computation of the viscous terms and SGS terms involves the use of first-order and second-order derivatives, which are discretized using fourth-order central finite-difference schemes.

2.3. Immersed boundary method

The use of the above high-order numerical method is facilitated by using a fixed structured staggered Cartesian grid (Shetty et al., 2010). In order to account for flow over or through complex shaped rigid or rotating bodies, an Immersed Boundary Method (IBM) is employed. Specifically, a mirroring of the fluid flow inside the solid body is used (Mark and van Wachem, 2008). The IBM requires a triangulated surface mesh for the objects we wish to flow over or through. The procedure begins with a computation of the surface normal for each surface point. Next, the structured Cartesian grid points are separated into two categories: inside or outside of the immersed body (IB) or bodies. For the solid points, ghost points (GPs) are defined as those having a neighbor inside the fluid region. The ghost points are projected into the fluid region, normal to the surface of the IB (using the previously computed normals). This results in a boundary point (BP) on the surface and an image point (IP) inside the fluid region (see Fig. 1). The value of the velocity at the boundary point $\overrightarrow{u}_{BP}$ is set to enforce the desired boundary condition at the IB surface. The value of the velocity at the IP $\overrightarrow{u}_{IP}$ is obtained by