MODELING 3-D COMPLIANT BLOOD FLOW WITH FOSLS

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ABSTRACT

Blood flow in large vessels is typically modeled using the Navier-Stokes equations for the fluid domain and elasticity equations for the vessel wall. As the wall deforms, additional complications are introduced because the shape of the fluid domain changes, necessitating the use of a re-mapping or re-griding process for the fluid region. Typically, this system (fluid, solid, mapping) is solved using an iterative approach in which the fluid, elastic, and mapping equations are solved in series until the iterations converge. We present a new approach based on multilevel minimization of the finite element approximation error using a least-squares (LS) norm. This approach allows for minimization of the error for the entire system or in selected parts. The multilevel LS approach overcomes many shortcomings of standard techniques. Most notably, the computational cost of solving the problem increases linearly with the degrees of freedom and the associated least-squares functional provides an *a posteriori* error measure. This paper compares the LS finite element approach to other popular numerical methods, specifically, the commercial package CFD-ACE. The focus of the comparison is on accuracy, computational cost, scalability (both parallel and serial), and flexibility. We show that the multilevel LS finite element apporach scales optimally (i.e., linearly in serial environments), while the other methods degrade substantially as the problem size increases.

INTRODUCTION

The mechanical coupling of a solid and fluid is important in a wide range of applications [1], from the coupling of an aircraft structure with the surrounding high Reynold's number fluid (aeroelasticity) to the compaction of a soft biofilm on a filter by a viscous, low Reynold's number flow. The mathematical characteristics of the problem also vary widely and no single approach can be applied to all fluid-solid problems. The focus here is on relatively low Reynold's number (<10,000), Newtonian fluids coupled with relatively low modulus materials, such as a soft tissue. In this regime, the mathematical characteristics of the equations for both fluid and solid are similar – the equations are elliptic (after implicit temporal discretization) and nonlinear. The biggest difference between the equations is that the elasticity equations for the solid are typically defined on a Lagrangian reference frame, which is based on the at-rest position of the material, and the fluid equations are based on the Eulerian reference frame.

There are three mathematical issues associated with coupled problems that we address in this paper. First, the equations for each individual domain (fluid or solid) are often nonlinear and, further, the problems are inherently nonlinear because the shape of the fluid domain is not known *a priori*--rather, it is determined in part by the deformation of the solid. Developing a method that can robustly handle nonlinearities is critical to solving coupled fluid-solid problems. Second, standard discretizations of the linearized Navier-Stokes and elasticity equations yields a matrix that is not positive definite, resulting in a linear system that is difficult to solve iteratively [2]. Further, standard iterative methods for this linear system do not scale optimally (i.e., the CPU time does not vary linearly with the number of unknowns). In this paper, a method that potentially scales optimally is explored. Third, the matching of stresses between the solid and fluid is critical for an accurate solution to the coupled problem. Therefore, the measurement of error, especially stress matching error, is critical to ensuring a stable solution. Error measurement also enables the use of adaptive refinement to reduce computational costs. In fact, the LS method described in the next section, FOSLS, provides a local sharp error measure for the coupled problem.

The techniques presented in this paper could be applied to a number of problems involving fluid and solid iteration. However, we focus on blood flow in large vessels since it is emerging as a standard fluid-solid problem. The most common technique for simulating blood flow in a compliant vessels is to begin by discretizing the fluid and solve on an initial mesh, solving for the displacement of the vessel wall assuming it to be a thin shell, to then move the fluid mesh, and, finally, repeat these three steps until convergence is achieved [3,4]. The method presented here uses a unified approach in that the fluid and structure are combined in a single solution stage. Only the movement of the mesh is performed in a separate calculation.

METHODS

The modeling of the blood flow—vessel wall coupled system requires the selection of differential equations for the fluid (blood) and solid (vessel wall). In large vessels, blood is frequently modeled as a Newtonian fluid using the Navier-Stokes equations [5]:

$$\begin{aligned} \rho(\mathbf{v}_t + \mathbf{v}\cdot\nabla\mathbf{v}) &= -\nabla p + \mu\nabla^2\mathbf{v} \\ \nabla\cdot\mathbf{v} &= 0 \end{aligned} \qquad (5,6)$$

The vessel wall displacement due to stress from blood flow is typically small [3], thus allowing the use of linear elasticity to model the vessel wall:

$$-\mu_E\nabla^2\mathbf{u} - (\lambda+\mu_E)\nabla\nabla\cdot\mathbf{u} = 0. \qquad (7)$$

Frequently, equation (7) is simplified further by modeling the vessel wall as a shell [3,4], but that simplification is not needed nor made here. Finally, the mesh or grid of the fluid region must be moved to account for the movement of the solid. Elliptic Grid Generation (EGG) is used here to map the deformed fluid domain back to the original computational grid. Using EGG, only a single grid is needed for the fluid, and the changing shape of the fluid domain is account for by solving *mapped* Navier-Stokes equations instead of equations (5,6) directly.

The basic idea behind FOSLS for solving a system of partial differential equations (i.e., Navier-Stokes, elasticity, and EGG) is to rewrite all equations as a first-order system and apply a least-squares 'energy' minimization principle. This reformulation must be done very carefully so that the resulting problem is well behaved in a physically meaningful way, and this can be difficult to accomplish for a given set of equations. However, the reformulation effort can be well worth the accompanying advantages, including its simplified framework for developing accurate discretizations (e.g., the 'inf-sup' condition does not apply allowing freedom in the choice of basis for each variable), optimal multigrid solver performance, and its sharp *a posteriori* error estimator that comes as a byproduct of the computation. To illustrate the basic FOSLS approach, consider again the Navier-Stokes equations (5,6), this time assumed to be steady-state for simplicity ($\mathbf{v}_t = \mathbf{0}$). Ignoring boundary conditions and other details for brevity, define the new matrix variable $\mathbf{V}$ as the gradient of $\mathbf{v}$. Since $\mathbf{V}$ is a gradient for each component of $\mathbf{v}$, its curl vanishes. This is written for simplicity as the equation $\nabla\times\mathbf{V} = 0$. Thus, the Navier-Stokes equations can be written as the following first-order system:

$$\begin{aligned} \mathbf{V} - \nabla\mathbf{v} &= 0 \\ -\mu\nabla\mathbf{V} + \rho(\mathbf{v}\cdot\mathbf{V}) + \nabla p &= 0 \\ \nabla\times\mathbf{V} &= 0 \\ \nabla(trace(\mathbf{V})) &= 0 \\ \nabla\cdot\mathbf{v} &= 0 \quad \text{(optional)} \end{aligned} \quad . \qquad (8, 9, 10, 11, 12)$$

We can now rewrite the first-order system as the problem of minimizing the following functional:

$$\begin{aligned} G(\mathbf{V},\mathbf{v},p) :=& \| \mathbf{V} - \nabla\mathbf{v} \|^2 + \| -\mu\nabla\mathbf{V} + \rho(\mathbf{v}\cdot\mathbf{V}) + \nabla p \|^2 \\ &+ \| \nabla\times\mathbf{V} \|^2 + \| \nabla(trace(\mathbf{V})) \|^2 + \| \nabla\cdot\mathbf{v} \|^2 \end{aligned}, \qquad (13)$$

where $\|\cdot\|$ denotes the L^2 norm. The FOSLS functional for the fully coupled elastic-fluid-EGG equation system is clearly much more complex than this functional for just the Navier-Stokes equations. What makes the minimization problem well posed is the property that the functional is equivalent to the square of the H^1 norm of the error [6]. Therefore, both smooth and "wiggly" error is exposed by the function – a significant advantage for coupled problems where wall stress is important.

To solve the coupled problem, there are many options available regarding the iterative strategy. For example, a single functional containing all of the first-order equations from the Navier-Stokes, elasticity, and EGG systems could be constructed. This functional would be significantly more complicated than equation (13), but it has the benefit that iterations only need to be performed on a single functional, which simplifies the iterative strategy. On the other extreme, 3 functionals could be formed that are all similar to equation (13). In this case, an outer iteration must be constructed to cycle between the 3 functionals (Navier-Stokes, elasticity, and EGG) until convergence is achieved. The option we chose is between these two extremes. We form one functional consisting of the Navier-Stokes and elasticity equations, and a second functional for just the EGG (mapping) equations. This approach has good convergence because the Navier-Stokes and elacticity equations are coupled in a single functional, but it does not suffer from an incorrect scaling that is likely when the EGG equations are also coupled [7]. A simple outer iteration between these two functionals, which are solved in an alternating series, is constructed, but one can envision more complex schemes where the remapping is only performed when a certain tolerance is exceeded. In all cases, the linear system resulting from a finite element discretization of the FOSLS functional is solved using a Conjugate Gradient solver with an Algebraic Multigrid Preconditioner (AMG/CG).

RESULTS

The first test problem is a simple straight tube of diameter 1 (dimensionless) and length 3. The walls of the tube have thickness 0.3, and the outer edge of the wall is fixed. The velocity at the inlet is normal to the surface and parabolic. The flow rate into the tube is periodic with a 1 sec period length. Over the first half of the period, the velocity is described by a half sine wave, and the flow is zero over the second half of the period. The stress between the fluid and the solid is matched along the interface, and the velocity is set to zero (no-slip) along the vessel wall. The elastic wall is allowed to compress and expand in the plane of the inlet by setting the tangential component of the normal stress to zero. Figure 1a shows the straight tube problem with no flow and the vessel wall in the at rest position. Figure 1b shows the flow and elastic deformation at the peak flow (0.25 sec. into a cycle). The vessel wall and pressure are only shown for a single plane passing vertically through the centerline for clarity. The vessel wall near the inlet of figure 1b is compressed due to the higher pressures found at the inlet. The pressure drop in the tube is approximately 8 (dimensionless) at peak flow.

(a)

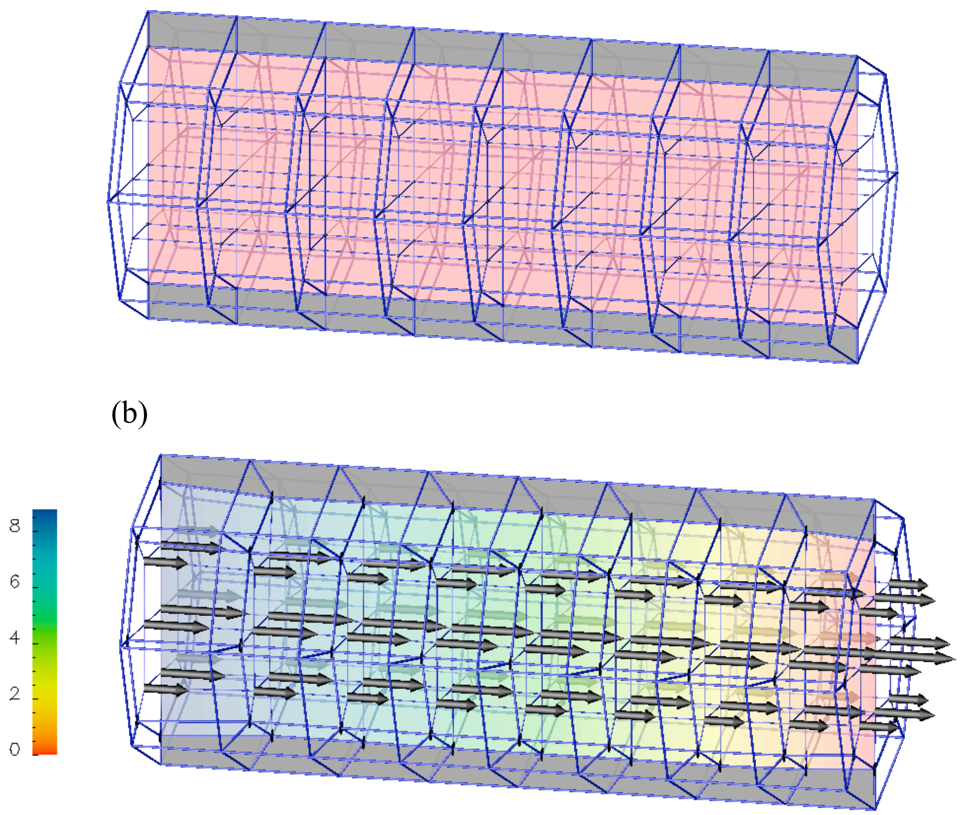


Figure 1. Flow through a straight tube with flexible walls. (a) No flow. (b) Peak flow.

The finite element mesh used to obtain the solution in Figure 1 is the coarsest mesh used in any of the simulation results presented. An implicit backward Euler time step of 0.02 was used in all results shown. Although this is a relatively small time step, it has the benefit of only requiring one outer iteration per time step. In other words, for each time step, the Navier-Stokes/elasticity equations were only solved once, and the EGG (mapping) equations were also solved only once. Further, despite the fact that both the Navier-Stokes and EGG equations are nonlinear, a stable solution was found with only a single linearization step (i.e., Newton step) each time the equations were solved. This is largely due to the accurate initial guess provided by the previous time step.

Figure 2 summarizes the numerical performance of the FOSLS finite element formulation with a AMG/CG solver on the coupled straight tube problem. The left axis illustrates the reduction in error with decreasing mesh size (increasing the number of degrees of freedom). Since a trilinear basis is used, the reduction is not extremely fast, but it is optimal for that particular basis. The more significant result is show on the right axis; the increase in CPU time as the problem size increases is linear (note that a log scale is used for clarity). As figure 2 shows, doubling the number of degrees of freedom results in only a doubling of the computational cost (i.e., optimal scalability).

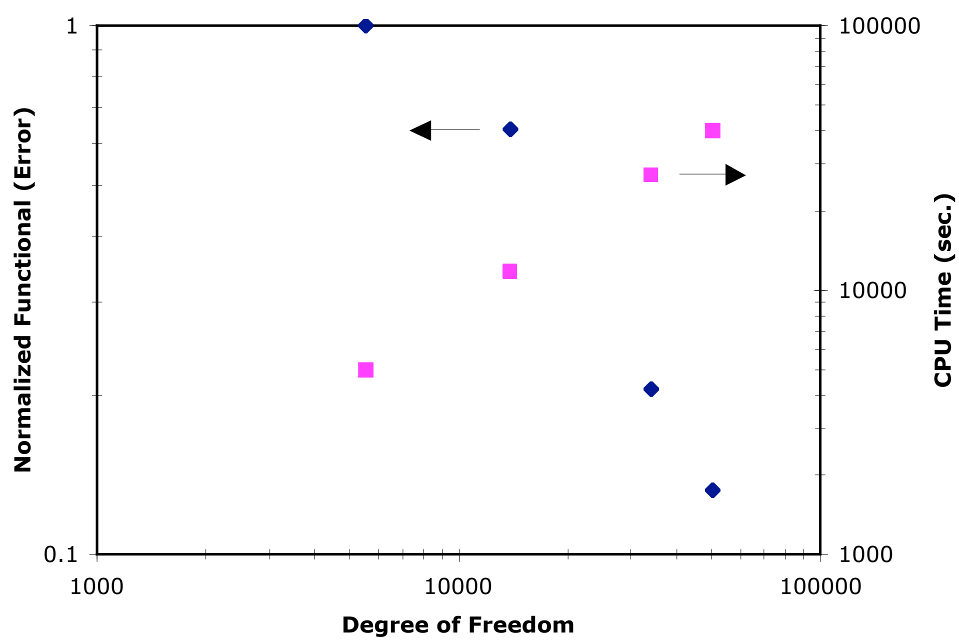
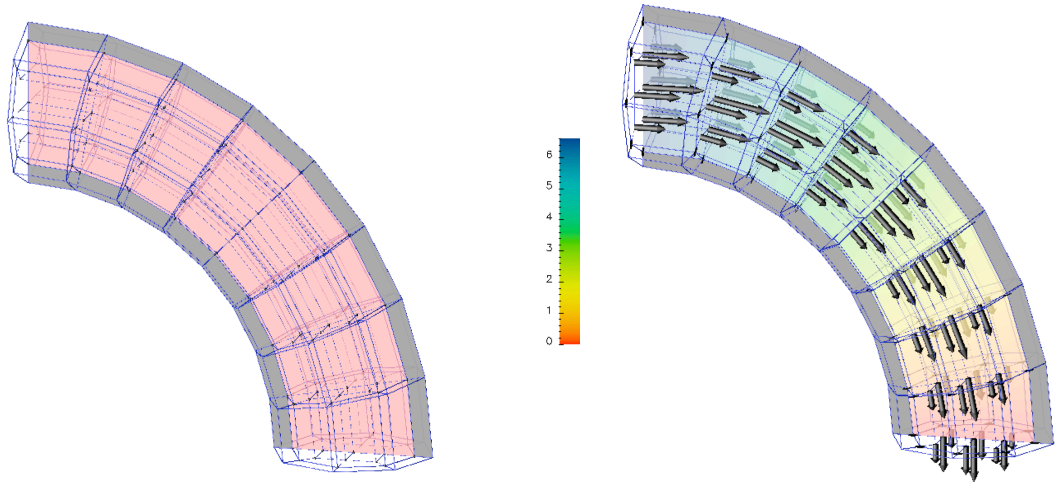


Figure 2. Numerical performance for the straight tube problem. The error (diamonds) is reduced at the expected rate as the mesh is refined, and, most significantly, the CPU time (squares) increases linearly with the problem size (optimal scaling).

The second test problem is designed to model the descending arch of the Aorta. The geometry is essentially a quarter circle with a tube diameter of 1.5cm and a centerline radius of curvature of 4 cm. Once again, the inlet flow is pulsatile with the pulse being described by a half sine wave. Figure 3(a) shows the at rest or no flow geometry of the descending aorta, and figure 3(b) shows the pressure drop, velocity, and wall displacement at peak flow. The vessel wall motion due to flow is small in the curved aorta simulation. In reality, there is wall motion due to the movement of the heart to which the aorta is attached [8], but this effect was not modeled here because accurate measurements are not available.



(a) (b)

Figure 3. Flow in the descending arch of the Aorta. (a) At rest vessel wall with no blood flow, and (b) the velocity, pressure drop, and displacement at peak flow.

The numerical performance of the AMG/CG solver and the FOSLS finite element discretization are summarized in Figure 4. The performance is consistent with that of the straight tube problem. The primary reason for this is that a multigrid solver can properly handle nonlinearities on coarse grids, allowing efficient and robust handling of complex, nonlinear problems.

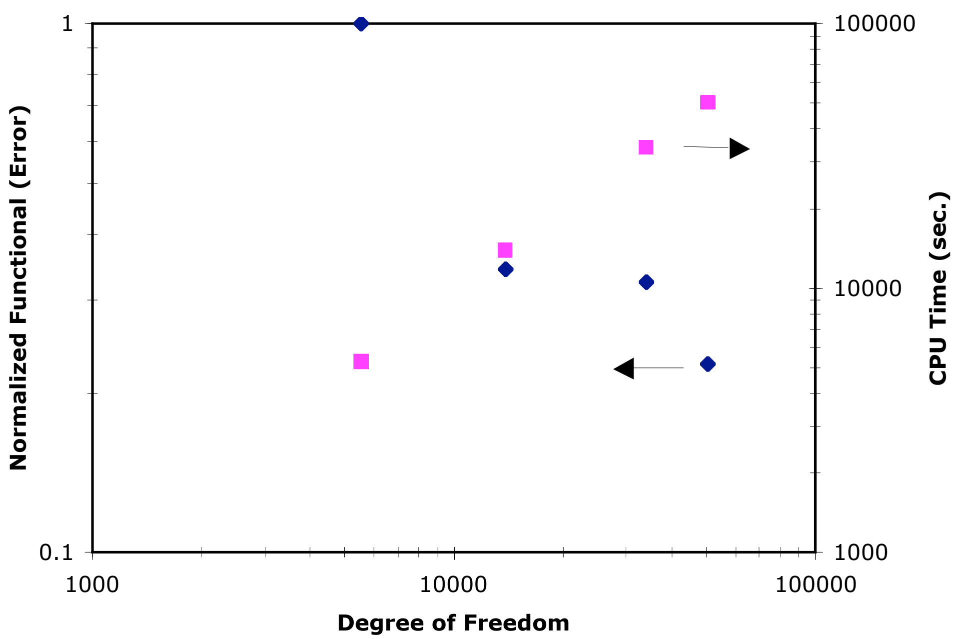


Figure 4. Numerical performance for the descending arch of the Aorta problem. The error (diamonds) is reduced at the expected rate with refinement, and the CPU time (squares) increases linearly with the problem size (optimal scaling).

DISCUSSION

As a comparison, we used the commercial code CFD-ACE™ to model the straight tube test problem with the half sine wave inlet condition. Using an implicit time step of 0.02 sec, CFD-ACE required 1.1 hours to solve the problem for a simple structured mesh. When the mesh was refined so that the problem size doubled, CFD-ACE required 3 hours to solve the problem. This observed approximate tripling of the computational time for a doubling of the problem size indicates that the solver used by CFD-ACE is not optimal. For comparison, we ran FOSLS simulations on the same problem using an equivalent PC with the same processor and slightly less memory. Using an identical implicit time step size of 0.02 seconds and spatial problem size that is essentially equivalent to the smaller problem, a FOSLS formulation with an AMG solver required only 0.7 hours. For a problem spatially equivalent to the larger problem (double the smaller problem), the FOSLS solver required only 1.5 hours, indicating optimal computational scaling. These results suggest that FOSLS is not only more efficient than CFD-ACE™ for small problems, but should become increasingly more so as the problem complexity increases.

CONCLUSIONS

The FOSLS finite element formulation can be successfully applied to the modeling of blood flow through compliant vessels. The formulation has 3 significant advantages over other approaches:

- used in conjunction with an AMG/CG iterative solver, the method achieves optimal scalability,
- multilevel methods permit the robust handling of nonlinearities on the coarse grid, and
- the FOSLS functional provides a sharp error measure.

These advantages have been illustrated for pulsatile flow in a straight tube problem and pulsatile flow through the descending arch of the Aorta.

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