

A Fully Implicit Domain Decomposition Based ALE Framework for Three-dimensional Fluid-structure Interaction with Application in Blood Flow Computation[☆]

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Abstract

Due to the rapid advancement of supercomputing hardware, there is a growing interest in parallel algorithms for modeling the full three dimensional interaction between the blood flow and the arterial wall. In [4], Barker and Cai developed a parallel framework for solving fluid-structure interaction problems in two dimensions. In this paper, we extend the idea to three dimensions. We introduce and study a parallel scalable domain decomposition method for solving nonlinear monolithically coupled systems arising from the discretization of the coupled system in an arbitrary Lagrangian-Eulerian framework with a fully implicit stabilized finite element method. The investigation focuses on the robustness and parallel scalability of the Newton-Krylov algorithm preconditioned with an overlapping additive Schwarz method. We validate the proposed approach and report the parallel performance for some

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patient-specific pulmonary artery problems. The algorithm is shown to be scalable with a large number of processors and for problems with millions of unknowns.

Keywords: fluid-structure interaction, blood flow simulation, restricted additive Schwarz, domain decomposition, fully implicit, monolithic coupling, parallel computing

1. Introduction

In order to understand computationally the sophisticated hemodynamics in human arteries, fluid-structure interaction (FSI) problems have received more and more attention in recent years [31, 34, 36]. In particular, researchers are increasingly interested in computational techniques for the coupled problem in full three dimensions, because these three-dimensional models provide results that can be used to quantify phenomena that are difficult to describe using simplified deformable wall models [16]. To include the effect of the deformable arterial wall in the FSI simulation, there exists a variety of methods to keep track of the fluid-structure coupling on the moving interface. The most popular choice is the arbitrary Lagrangian-Eulerian (ALE) framework [15, 17, 30]. Within the ALE framework, the displacement of the fluid domain is introduced as a third field of solution variables in the coupled system, so that coupling conditions are guaranteed to be satisfied on the fluid-structure interface. Other approaches in the literatures, to name a few, include the space-time formulation [6, 37], the immersed boundary method [19, 38], and the coupled momentum method [16, 43].

In this paper, we adopt the ALE framework. The arterial wall is modeled

as a linear elastic structure in the Lagrangian description and the blood flow is assumed to be a Newtonian fluid governed by the incompressible Navier-Stokes equations in the ALE form. In addition, an auxiliary Laplace equation is used to model the deformation of the moving fluid domain. We use the monolithic approach to couple the fluid, the structure, and the moving domain subsystems in a single system as in [4]. The tight coupling provided by the monolithic approach eliminates the so-called added-mass effect [8] and shows better robustness to physical parameters [6]. But solving monolithically coupled problems is a rather challenging task. The new equation introduced by the ALE framework and its dependence on the solution introduce further complexities and nonlinearities. To solve the fully coupled system in a reasonable time requires the development of solution algorithm that is not only computationally efficient, but also suitable for high performance computers with a large number of processors [18].

In this work, we focus on developing a class of Newton-Krylov method (NK) with an overlapping restricted additive Schwarz preconditioner for solving the nonlinear systems arising from fully coupled FSI problems, with emphasis on the robustness and the parallel scalability. In our method, a finite element method with time dependent stabilization is used to discretize the coupled problem in space and a fully implicit backward difference scheme is used for the temporal discretization. The resulting discretized system is highly nonlinear because of the convective term of the Navier-Stokes equations and the dependency of the solution on the displacement of the moving fluid mesh. To handle these nonlinearities, in [2, 9] some linearization techniques based on a fixed point algorithm were studied, in which the nonlinear

dependence on the moving mesh and/or the convective term is linearized by an extrapolation from the solution of the previous time step. These semi-implicit treatments work well in most cases, but may not be stable when the time step size is large. In the present paper, we treat all terms in the system implicitly, which leads to a much more stable scheme. We use an inexact Newton method to solve the large nonlinear algebraic system, within which a Krylov subspace method is used to solve the analytically computed Jacobian systems. In NK, the most crucial question is how to develop an effective and efficient preconditioner for the linear Jacobian systems. In [24], an algebraic multigrid preconditioner is used. In [9], a class of preconditioners based on the block-structure of an approximate Jacobian system is introduced. In our work, we employ a monolithic overlapping restricted additive Schwarz preconditioner to speed up the convergence of a Krylov subspace method. NK together with the additive Schwarz preconditioner has been successfully used in solving various problems and shown good parallel scalability, for example, [21, 25] for fluid dynamics problems, [42] for atmospheric flow problems, and [4] for two-dimensional FSI problems. In this work, we extend the algorithms to solve the fully implicit, fully coupled, three-dimensional FSI problems.

The rest of the paper is organized as follows. In Section 2, we describe the formulation and the discretization of the FSI problem. In Section 3, we present the Newton-Krylov-Schwarz method for solving the fully coupled nonlinear system. In Section 4, we demonstrate the effectiveness and report the parallel performance of the algorithm by showing some numerical results using different geometries. Finally, we provide some concluding remarks in Section 5.

2. Mathematical models and a fully implicit, monolithic finite element discretization

When blood flows in an artery, the elastic wall deforms in response to the blood pressure and other external forces, which in turn changes the shape of the fluid domain. We model the fluid-structure interaction by using a coupled system of nonlinear equations. For the arterial wall, we consider a linear elastic model. For the fluid, we use the incompressible Navier-Stokes equations, assuming that blood is Newtonian in large arteries. To address the moving fluid domain, an additional field and the corresponding governing equations are introduced for modeling the domain deformation. In all, the monolithic FSI model is described by three components: the elastic wall structure, the fluid, and the motion of the fluid domain. The external force from the surrounding tissues is modeled by a stabilization term in the elasticity equation, and the gravitational force is ignored.

Let $\Omega^t = \Omega_f^t \cup \Omega_s^t$ be the combined fluid subdomain $\Omega_f^t \subset R^3$ and structure subdomain $\Omega_s^t \subset R^3$ at time t . The initial configuration of the domain is defined as $\Omega^0 = \Omega_f^0 \cup \Omega_s^0$ when $t = 0$. $\Gamma_w^t = \partial\Omega_f^t \cap \partial\Omega_s^t$ represents the interface between the fluid and structure subdomains, and Γ_w^0 is the corresponding interface in the initial configuration. We model the structure problem with a linear elasticity equation, using the Lagrangian frame of reference. The displacement \mathbf{x}_s of the structure at the reference configuration is assumed to satisfy

$$\rho_s \frac{\partial^2 \mathbf{x}_s}{\partial t^2} + \alpha \frac{\partial \mathbf{x}_s}{\partial t} - \nabla \cdot \sigma_s = \mathbf{f}_s \quad \text{in } \Omega_s^0, \quad (1)$$

where ρ_s is the density of the structure, and $\sigma_s = \lambda_s(\nabla \cdot \mathbf{x}_s)I + \mu_s(\nabla \mathbf{x}_s + \nabla \mathbf{x}_s^T)$

is the Cauchy stress tensor. The Lamé parameters λ_s and μ_s are related to the Young's modulus E and the Poisson ratio ν_s by $\lambda_s = \nu_s E / ((1 + \nu_s)(1 - 2\nu_s))$ and $\mu_s = E / (2(1 + \nu_s))$. In [4, 5], two-dimensional blood flows in compliant arteries were successfully simulated without the stabilization of the elasticity equation; i.e. $\alpha = 0$. In other words, the impact of surrounding tissues is not considered in 2D, and the instability problem does not show up. However, according to numerical experiments conducted by us and others, in three-dimensional simulations, the blood flow and the elasticity waves inside the artery may become unstable sometimes, without a carefully chosen stability constant α . Following [33, 37], a mass-proportional damping coefficient α is considered in our formulation to represent the damping effect of the surrounding tissue on the artery. Other choice concerning the surrounding tissue effects can also be found in [10] which imposes special boundary conditions on the external arterial wall.

To model the fluid in the moving domain Ω_f^t , we use the ALE framework. More detailed applications of ALE can be found in [15, 17, 30] and references therein. We assume that the displacement of the fluid domain \mathbf{x}_f at the reference configuration Ω_f^0 satisfies a harmonic extension of the moving fluid-structure interface,

$$\Delta \mathbf{x}_f = 0 \quad \text{in } \Omega_f^0.$$

This choice of the model for the moving fluid domain is not unique and not based directly on the physics of the FSI problem. Other choices are available [22, 26]. Based on our experiments, this simple scheme performs well, maintaining good conditioning of elements even under relatively large deformation.

Next, we define an ALE mapping A_t from Ω_f^0 to Ω_f^t :

$$A_t : \Omega_f^0 \rightarrow \Omega_f^t, \quad A_t(\mathbf{Y}) = \mathbf{Y} + \mathbf{x}_f(\mathbf{Y}), \quad \forall \mathbf{Y} \in \Omega_f^0,$$

where \mathbf{Y} is referred to as the ALE coordinates. The incompressible Navier-Stokes equations defined on the moving domain Ω_f^t are then written in the ALE form as

$$\begin{aligned} \rho_f \frac{\partial \mathbf{u}_f}{\partial t} \Big|_Y + \rho_f [(\mathbf{u}_f - \omega_g) \cdot \nabla] \mathbf{u}_f - \nabla \cdot \sigma_f &= 0 \quad \text{in } \Omega_f^t, \\ \nabla \cdot \mathbf{u}_f &= 0 \quad \text{in } \Omega_f^t, \end{aligned}$$

where ρ_f is the fluid density, \mathbf{u}_f is the fluid velocity, and $\sigma_f = -p_f I + \mu_f(\nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T)$ is the Cauchy stress tensor. $\omega_g = \partial \mathbf{x}_f / \partial t$ is the velocity of the moving domain and Y indicates that the time derivative is taken with respect to the ALE coordinates.

In addition to the equations above, three coupling conditions are needed at the fluid-structure interface. Firstly, we require the continuity of the velocities on the interface,

$$\mathbf{u}_f = \frac{\partial \mathbf{x}_s}{\partial t}. \quad (2)$$

Secondly, we require the continuity of the traction forces on the interface,

$$\sigma_s \cdot \mathbf{n}_s = -\sigma_f \cdot \mathbf{n}_f, \quad (3)$$

where \mathbf{n}_s , \mathbf{n}_f are unit normal vectors for the structure and fluid domains. Thirdly, we require that the motion of the fluid domain follows the structure displacement, so that the structure can maintain a Lagrangian description,

$$\mathbf{x}_f = \mathbf{x}_s. \quad (4)$$

Note that the fluid equations are first-order in time, but the elasticity equation is second-order in time. By introducing the structure velocity $\dot{\mathbf{x}}_s$ as an additional unknown variable, we can rewrite the structure momentum equation (1) as a first-order system of equations. We define the function space of the structure problem as

$$X = \{ \mathbf{x}_s \in H^1([0, T]; [H^1(\Omega_s^0)]^3) : \mathbf{x}_s(\cdot, t) = 0 \text{ on } \Gamma_s \},$$

where Γ_s is the fluid-structure interface. The corresponding weak form is stated as follows: Find $\mathbf{x}_s \in X$ and $\dot{\mathbf{x}}_s \in X$ such that $\forall \phi_s \in X$ and $\forall \varphi_s \in X$,

$$\begin{aligned} B_s(\{\mathbf{x}_s, \dot{\mathbf{x}}_s\}, \{\phi_s, \varphi_s\}; \sigma_f) &= \rho_s \frac{\partial}{\partial t} \int_{\Omega_s^0} \dot{\mathbf{x}}_s \cdot \phi_s \, d\Omega + \alpha \int_{\Omega_s^0} \dot{\mathbf{x}}_s \cdot \phi_s \, d\Omega \\ &+ \int_{\Omega_s^0} \nabla \phi_s : \sigma_s \, d\Omega + \int_{\Gamma_w^t} \phi_f \cdot (\sigma_f \cdot \mathbf{n}_f) \, ds - \int_{\Omega_s^0} \mathbf{f}_s \cdot \phi_s \, d\Omega \quad (5) \\ &+ \int_{\Omega_s^0} \left(\frac{\partial \mathbf{x}_s}{\partial t} - \dot{\mathbf{x}}_s \right) \cdot \varphi_s \, d\Omega = 0. \end{aligned}$$

It is important to emphasize that the coupling condition (3) are implicitly enforced as part of (5) by the relation

$$\int_{\Gamma_w^0} \phi_s \cdot (\sigma_s \cdot \mathbf{n}_s) \, ds + \int_{\Gamma_w^t} \phi_f \cdot (\sigma_f \cdot \mathbf{n}_f) \, ds = 0.$$

Here the test function ϕ_f will be defined below.

The function spaces of the fluid subproblem are time dependent, and the solution of the structure subproblem provides an essential boundary condition for the fluid subproblem by (2). We define the trial and weighting function spaces as:

$$\begin{aligned} V &= \left\{ \mathbf{u}_f \in H^1([0, T]; [H^1(\Omega_f^t)]^3) : \mathbf{u}_f(\cdot, t) = g \text{ on } \Gamma_i, \mathbf{u}_f(\cdot, t) = \frac{\partial \mathbf{x}_s}{\partial t} \text{ on } \Gamma_t^w \right\}, \\ V_0 &= \{ \mathbf{u}_f \in H^1([0, T]; [H^1(\Omega_f^t)]^3) : \mathbf{u}_f(\cdot, t) = 0 \text{ on } (\Gamma_i \cup \Gamma_t^w) \}, \\ P &= \{ p_f(\cdot, t) \in L^2([0, T]; L^2(\Omega_f^t)) \}. \end{aligned}$$

The weak form of the fluid problem reads: Find $\mathbf{u}_f \in V$ and $p_f \in P$ such that $\forall \phi_f \in V_0$ and $\forall \psi_f \in P$,

$$\begin{aligned} B_f(\{\mathbf{u}_f, p_f\}, \{\phi_f, \psi_f\}; \mathbf{x}_f) &= \rho_f \int_{\Omega_t^f} \frac{\partial \mathbf{u}_f}{\partial t} \Big|_Y \cdot \phi_f \, d\Omega - \int_{\Omega_t^f} p_f (\nabla \cdot \phi_f) \, d\Omega \\ &+ \rho_f \int_{\Omega_t^f} [(\mathbf{u}_f - \omega_g) \cdot \nabla] \mathbf{u}_f \cdot \phi_f \, d\Omega + 2\mu_f \int_{\Omega_t^f} \epsilon(\mathbf{u}_f) : \epsilon(\phi_f) \, d\Omega \\ &+ \int_{\Omega_t^f} (\nabla \cdot \mathbf{u}_f) \psi_f \, d\Omega = 0, \end{aligned}$$

where $\epsilon(\mathbf{u}_f) = (\nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T)/2$. The weak form of the domain movement problem reads: Find $\mathbf{x}_f \in Z$ such that $\forall \phi_m \in Z_0$,

$$B_m(\mathbf{x}_f, \phi_m) = \int_{\Omega_f^0} \nabla \mathbf{x}_f : \nabla \phi_m \, d\Omega = 0.$$

And the function spaces are defined as

$$\begin{aligned} Z &= \{\mathbf{x}_f \in [H^1(\Omega_f^0)]^3 : \mathbf{x}_f = \mathbf{x}_s \text{ on } \Gamma_w^0, \mathbf{x}_f = 0 \text{ on } \Gamma_i \cup \Gamma_o\}, \\ Z_0 &= \{\mathbf{x}_f \in [H^1(\Omega_f^0)]^3 : \mathbf{x}_f = 0 \text{ on } \Gamma_i \cup \Gamma_o \cup \Gamma_w^0\}. \end{aligned}$$

We discretize the weak problem in space with a conforming moving finite element method, consisting of quasi-uniform unstructured P1-P1 stabilized elements for the fluid, P1 elements for the structure and P1 elements for the fluid domain motion. The mesh is generated in a way so that the interface between the fluid and structure is aligned with the mesh, see Figure 1. In other words, the interface does not cut through any elements. But such a restriction is not followed later when we partition the mesh to define the domain decomposition solver. We denote the finite element subspaces $X_h, V_h, V_{h,0}, P_h, Z_h, Z_{h,0}$ as the counterparts of their infinite dimensional subspaces. Because the fluid problem requires that the pair V_h and P_h satisfy the LBB

inf-sup condition, additional stabilization terms are needed in the formulation with equal-order interpolation of the velocity and the pressure as described in [35, 40]. The semi-discrete stabilized finite element formulation for the fluid problem reads as follows: Find $\mathbf{u}_f \in V_h$ and $p_f \in P_h$, such that $\forall \phi_f \in V_{h,0}$ and $\forall \psi_f \in P_h$,

$$B(\{\mathbf{u}_f, p_f\}, \{\phi_f, \psi_f\}; \mathbf{x}_f) = 0,$$

with

$$\begin{aligned} & B(\{\mathbf{u}_f, p_f\}, \{\phi_f, \psi_f\}; \mathbf{x}_f) \\ &= B_f(\{\mathbf{u}_f, p_f\}, \{\phi_f, \psi_f\}; \mathbf{x}_f) + \sum_{K \in \mathcal{T}_f^h} (\nabla \cdot \mathbf{u}_f, \tau_c \nabla \cdot \phi_f)_K \\ &+ \sum_{K \in \mathcal{T}_f^h} \left(\left. \frac{\partial \mathbf{u}_f}{\partial t} \right|_Y + (\mathbf{u}_f - \omega_g) \cdot \nabla \mathbf{u}_f + \nabla p_f, \tau_m ((\mathbf{u}_f - \omega_g) \cdot \nabla \phi_f + \nabla \psi_f) \right)_K \\ &+ \sum_{K \in \mathcal{T}_f^h} (\bar{\mathbf{u}}_{\mathbf{f}} \cdot \nabla \mathbf{u}_f, \phi_f)_K + \sum_{K \in \mathcal{T}_f^h} (\bar{\mathbf{u}}_{\mathbf{f}} \cdot \nabla \mathbf{u}_f, \tau_b \bar{\mathbf{u}}_{\mathbf{f}} \cdot \nabla \phi_f)_K, \end{aligned}$$

where $\mathcal{T}_f^h = \{K\}$ is the given unstructured tetrahedral fluid mesh, and $\bar{\mathbf{u}}_{\mathbf{f}}$ is the conservation-restoring advective velocity introduced in [35],

$$\bar{\mathbf{u}}_{\mathbf{f}} = -\tau_m \left(\left. \frac{\partial \mathbf{u}_f}{\partial t} \right|_Y + (\mathbf{u}_f - \omega_g) \cdot \nabla \mathbf{u}_f + \nabla p_f \right).$$

The stabilization parameters τ_m , τ_c and τ_b are defined as in [6] and similar stabilization parameters are used in [16, 39] for some problems defined on a

fixed mesh, where

$$\begin{aligned}\tau_m &= \frac{1}{\sqrt{\frac{4}{\Delta t^2} + (\mathbf{u}_f - \omega_g) \cdot G(\mathbf{u}_f - \omega_g) + 36 \left(\frac{\mu_f}{\rho_f}\right)^2 G : G}}, \\ \tau_c &= \frac{1}{8\tau_m \text{tr}(G)}, \\ \tau_b &= \frac{1}{\sqrt{\bar{\mathbf{u}}_f \cdot G \bar{\mathbf{u}}_f}}.\end{aligned}$$

Here $G_{ij} = \sum_{k=1}^3 \frac{\partial \xi_k}{\partial x_i} \frac{\partial \xi_k}{\partial x_j}$ denotes the covariant metric tensor, which may be identified with the element length scale [39]. $\frac{\partial \xi}{\partial \mathbf{x}}$ represents the inverse Jacobian of the mapping between the reference and the physical domain. The term $4/\Delta t^2$ in τ_m is important only for time dependent problems, and is dropped for steady-state computations.

We form the finite dimensional fully coupled FSI problem as follows: Find $x_s \in X_h$, $\dot{x}_s \in X_h$, $u_f \in V_h$, $p_f \in P_h$ and $x_f \in Z_h$ such that $\forall \phi_s \in X_h$, $\forall \varphi_s \in X_h$, $\forall \phi_f \in V_{h,0}$, $\forall \psi_f \in P_h$, and $\forall \phi_m \in Z_{h,0}$,

$$B_s(\{x_s, \dot{x}_s\}, \{\phi_s, \varphi_s\}; \sigma_f) + B(\{u_f, p_f\}, \{\phi_f, \psi_f\}; x_f) + B_m(x_f, \phi_m) = 0. \quad (6)$$

The finite element formulations for each of the three subproblems have been validated. In the later section, we will validate through numerical experiments the correctness of the coupled formulation including all three components, as well as the coupling conditions.

By using the same time-stepping scheme for both the fluid and the structure. The semi-discrete system (6) is further discretized in time with a second-order backward differentiation formula (BDF2). That is, for a given semi-discrete system

$$\frac{dx}{dt} = \mathcal{L}(x),$$



Figure 1: Example finite element mesh for the fluid-structure interaction problem (top). The mesh is generated so that the interface between the fluid and structure is aligned with the mesh. The elements of the fluid (bottom left) and the elements of the structure (bottom right) conform on the interface.

the BDF2 scheme

$$x^n - \frac{4}{3}x^{n-1} + \frac{1}{3}x^{n-2} = \frac{2\Delta t}{3}\mathcal{L}(x^n)$$

is employed for the time integration. Here x^n represents the value of x at the n^{th} time step with a fixed time step size Δt .

The temporal discretization scheme is fully implicit, at each time step, we obtain the solution $x^n = (u_f, p_f, x_f, x_s, \dot{x}_s)$ at the n^{th} time step from the previous two time steps by solving a sparse, nonlinear algebraic system

$$\mathcal{F}_n(x^n) = 0, \tag{7}$$

where x^n corresponds to the nodal values of the fluid velocity \mathbf{u}_f , the fluid pressure p_f , the fluid mesh displacement \mathbf{x}_f , the structure displacement \mathbf{x}_s and the structure velocity $\dot{\mathbf{x}}_s$ at the n^{th} time step. For simplicity, we ignore the script n for the rest of the paper.

We note that \mathcal{F} is a highly nonlinear function, where the nonlinearities come from the convective term of the Navier-Stokes equations, the stabilization terms and the dependency on the displacement of the moving fluid mesh. In our fully implicit scheme, all the terms of the equations are treated implicitly instead of explicitly or semi-implicitly. This leads to a more stable and robust scheme, but the corresponding nonlinear systems (7) are quite difficult to solve because of the different characteristics their components have. In the fluid part of \mathcal{F} , there are 4 unknowns per mesh point, in the moving mesh part there are 3 unknowns per mesh point, and in the structure part there are 6 unknowns per mesh point. The equations for the fluid is time-dependent, nonlinear parabolic-like, the equations for the moving mesh are elliptic type, and the equations for the structure are time dependent linear

hyperbolic-like. The stiffness of the system is different in the fluid part and the structure part of the computational domain depending on the viscosity coefficient of the flow and the wall.

3. A monolithic nonlinear solver for the coupled system of equations

In this section we introduce an overlapping domain decomposition method for solving the coupled multi-physics system (7). The method is well studied for each individual component of the problem, namely the incompressible Navier-Stokes equation [25], the linear elasticity equation [28], the elliptic moving mesh equation [7]. In a recent paper [4], it was extended to the coupled system in two-dimensional space, here we further extend it to a full three-dimensional problem. To design an algorithm for (7) that is highly scalable in terms of the total compute time, many important factors need to be taken into consideration. The basic components of the algorithm are not new, but to arrive at the best combination, we consider not only the properties of the nonlinear system, the properties of the domain decomposition methods, but also the software and hardware of our computational environment.

In our Newton-Krylov-Schwarz approach, the nonlinear FSI system (7) is solved via the inexact Newton method with a cubic line search technique [13, 14]. To obtain the new solution $x^{(k+1)}$ at each Newton step, the Newton correction $s^{(k)}$ is approximated by solving a right-preconditioned Jacobian system with a Krylov subspace method, GMRES [32]

$$J_k M_k^{-1} M_k s^{(k)} = -\mathcal{F}(x^{(k)}), \quad (8)$$

where J_k is the Jacobian matrix evaluated at current solution $x^{(k)}$ and M_k^{-1} is a restricted additive Schwarz preconditioner [7]. The evaluation of the Jacobian J_k of the fully coupled system is non-trivial, especially for three-dimensional problems. As a result, most researchers choose to approximate the Jacobian by ignoring certain terms. The difficulty lies in the evaluation of the cross derivatives; e.g. the derivatives of the fully coupled system with respect to the mesh movement. One solution is to use a finite difference approximation to calculate the cross derivatives [23], but such approximation is required at each Newton iteration and may drastically increase the overall compute time. Another solution is to use a computationally inexpensive approximation of the Jacobian [20], but this may deteriorate the overall convergence. In our implementation, we compute the Jacobian analytically including all those cross derivatives. There are 66 derivatives at some of the grid points, so the task of hand-calculating these derivatives is time-consuming. However, this is a worthwhile excise since it saves many Newton iterations, and can be used to provide a better preconditioner for the Jacobian systems. We remark that, the robustness of Newton method is often not guaranteed when the Jacobian is approximately computed.

Another critically important component of the overall solver is the preconditioner, without which the iterative Jacobian solver (8) would not converge well, and as a result, the outer inexact Newton may not converge well either. To define the Schwarz preconditioner, we first partition the finite element mesh \mathcal{T}_h , constructed for the initial configuration, into non-overlapping subdomains Ω_ℓ^h , $\ell = 1, \dots, N$, where the number of subdomains N is always the same as the number of processors np . Then, each subdomain Ω_ℓ^h is extended

to an overlapping subdomain $\Omega_\ell^{h,\delta}$, where δ is an integer indicating the level of overlap; see Figure 2 for an example. The criteria of partition inherit from [4], where the two-dimensional meshes were studied. The partition is element-based and the degrees of freedom defined at a mesh point is taken into account to ensure load balancing; i.e., each subdomain has more or less the same number of unknowns. The decomposition of the mesh is completely independent of which physical variables are defined for a given mesh point. A subdomain may contain both fluid and structure elements.

We define the restriction operator R_ℓ as a mapping that maps the global vector of unknowns in Ω^h to those belonging to an overlapping subdomain $\Omega_\ell^{h,\delta}$. If n is the total number of unknowns in Ω^h and n_ℓ^δ is the number of unknowns in $\Omega_\ell^{h,\delta}$, then R_ℓ is an $n_\ell^\delta \times n$ sparse matrix. We construct a subdomain Jacobian by $B_\ell = R_\ell J_k R_\ell^T$, which is a restriction of the Jacobian matrix J_k to the subdomain $\Omega_\ell^{h,\delta}$. The restricted additive Schwarz preconditioner is defined by

$$M_k^{-1} = \sum_{\ell=1}^N (R_\ell^0)^T B_\ell^{-1} R_\ell,$$

where R_ℓ^0 is the restriction to the degrees of freedom in the non-overlapping subdomain Ω_ℓ^h . In the restricted additive Schwarz preconditioner, the overlapping regions between the overlapping subdomains are used to provide information to the subdomain solve, but the results of computation in the overlapping regions are not considered in the prolongation procedure in order to reduce the communication cost when implemented on parallel computers.

At each Newton step, the multiplication of M_k^{-1} with a vector r inside

the GMRES loop can be computed in the following two steps,

$$z_\ell = B_\ell^{-1}(R_\ell r), \ell = 1, \dots, N \quad (9)$$

$$M_k^{-1}r = \sum_{\ell=1}^N (R_\ell^0)^T z_\ell. \quad (10)$$

In the parallel implementation, on each processor, either a direct or an iterative approach can be used to solve the subdomain Jacobian systems (9). In our application, we use a sparse LU incomplete factorization based direct method. LU factorization can be computationally expensive if the subdomain problem is large, which often happens when the number of processors is relatively small. One possible approach to improve the efficiency of LU factorization is to control the level of fill-ins in the incomplete factorization. There are two types of ILU factorizations. The popular point-wise ILU works well for matrices arising from scalar partial differential equations, but sometimes fails for coupled multi-physics problems. We choose to use a point-block version of ILU, where we group all physical components associated with a mesh point as a block. By using the point-block version, we can improve considerably the robustness of the subdomain preconditioner, and at the same time improve the cache performance of the computation. The inverse of the small point-block matrix on the diagonal of the large matrix is computed exactly before the ILU factorization is carried out.

4. Numerical results

In this section, we report some numerical results of the proposed fully coupled FSI solver by simulating some blood flows in three-dimensional compliant arteries. We first validate the correctness of our solver by testing on a

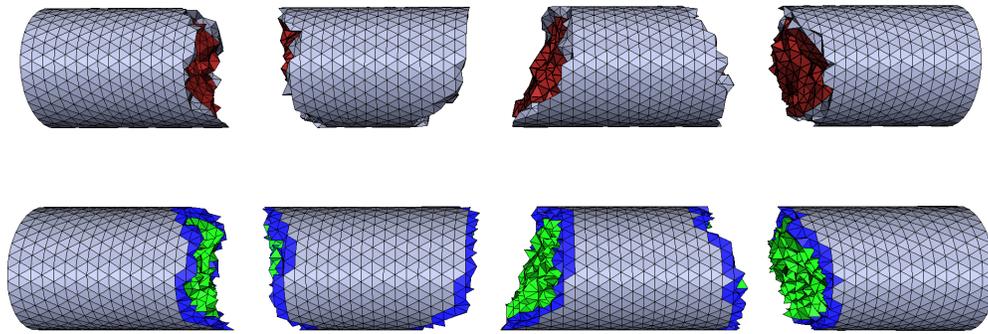


Figure 2: Example partition of the domain into 4 subdomains by using ParMETIS. The fluid elements and structure elements are marked with different colors. The top figure shows the partition into non-overlapping subdomains, and the bottom represents a corresponding partition into overlapping subdomains with $\delta = 2$. The shaded elements in blue and green represent the corresponding fluid elements and structure elements extended from the non-overlapping subdomains.

well-understood benchmark problem, then investigate the numerical behavior and parallel performance of our solver with two complex branching geometries derived from clinical data provided by colleagues at the University of Colorado Medical School. Our solver is implemented on top of the Portable Extensible Toolkit for Scientific computing (PETSc) library [3]. Mesh generations are carried out by CUBIT of Sandia National Laboratories [1] and mesh partitions are obtained with ParMETIS of University of Minnesota [27]. All computations are performed on the Dell PowerEdge C6100 Cluster at the University of Colorado Boulder.

4.1. A benchmark case

The setup of the benchmark 3D FSI problem consists of a straight cylinder representing the fluid domain with length 5 cm and radius 0.5 cm, and the surrounding wall with thickness 0.1 cm. A constant traction $\sigma_f \cdot \mathbf{n} = 1.33 \cdot 10^4 \text{ dynes/cm}^2$ is imposed on the inlet boundary for 3 ms. A zero traction condition is applied to the fluid at the outlet boundary. The fluid is characterized with viscosity $\mu_f = 0.03 \text{ g/(cm s)}$, and density $\rho_f = 1.0 \text{ g/cm}^3$. The Young's modulus $E = 3 \cdot 10^6 \text{ g/(cm s}^2)$, the Poisson ratio $\nu_s = 0.3$, and the structure density $\rho_s = 1.2 \text{ g/cm}^3$ are the parameters of the structure model. The damping parameter α is set to be zero in this case.

The fluid and the structure are initially at rest and the simulation is run for a total time of 10 ms with a time step size $\Delta t = 0.1 \text{ ms}$. The simulation proceeds to the next time step when the relative residual of the nonlinear system is less than 10^{-6} . The stopping criterion for the linear solver is when the preconditioned residual is decreased by a factor of 10^{-6} . To validate the correctness of the coupled spatial and temporal discretization scheme, we

run a simulation on a mesh with $2.41 \cdot 10^6$ elements and $3.08 \cdot 10^6$ degrees of freedom, and show the computed fluid pressure and the structure deformation at $t = 2.5, 5.0, 10.0$ ms in Figure 3. Our computed results are similar to the published results [12, 15]. The pressure wave propagation along the cylinder is observed. The wall structure deforms in response to the propagation of the pressure pulse, which is a key evidence of the fluid-structure interaction.

We next study the parallel performance and scalability of our fully coupled solver for the benchmark problem. We report the average compute time and the nonlinear iteration count per time step, as well as the average GMRES iterations per Newton step in the experiments, where the documented results are average values over the first 10 time steps. As shown in Figure 4, our algorithm shows excellent strong scalability. Based on the tests with two different meshes consisting of $1.25 \cdot 10^6$ and $3.08 \cdot 10^6$ degrees of freedom, the parallel speedup is shown to be nearly linear with up to 2048 processors. Although there is a mild growth in the number of GMRES iterations, the compute time is almost halved as we double the number of processors.

In an overlapping Schwarz preconditioner, the choice of subdomain solver has a significant impact to the overall performance. In Table 1, we show the results obtained using several different subdomain solvers including a point-block LU (BLU) and point-block ILU with $l = 1, 2$ levels of fill-ins (BILU(l)), and the standard pointwise sparse LU. When LU and BLU are used, the subdomain problem is solved exactly and the number of GMRES iterations is the smallest comparing with inexact subdomain solvers. However, in terms of the total compute time, BLU is always faster, in particular, when the number of processors is relatively small. In sparse matrix factorizations, the

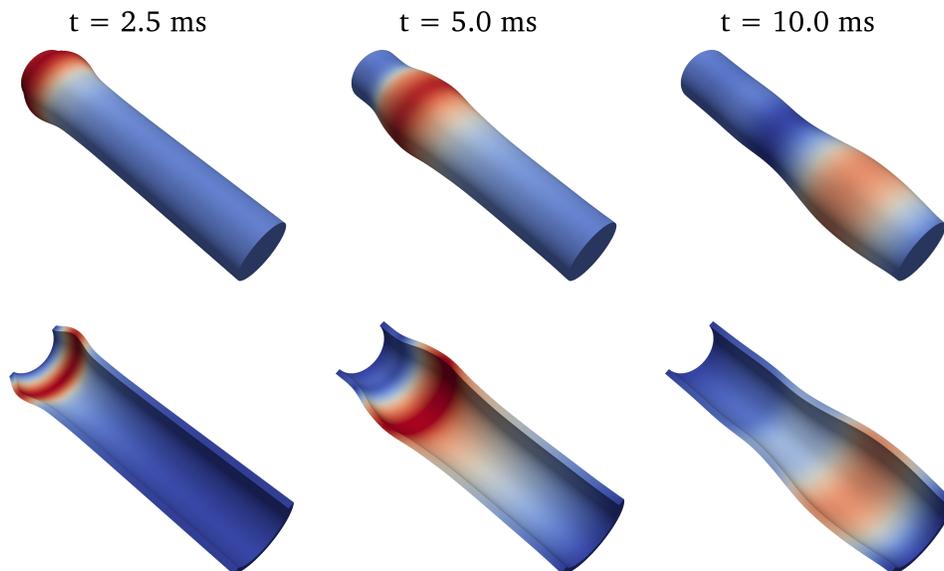


Figure 3: Pressure wave propagation (top row) and structure deformation (bottom row) for the straight cylinder case. The simulation is run on a mesh with $2.41 \cdot 10^6$ elements and $3.08 \cdot 10^6$ degrees of freedom. The deformation is amplified by a factor of 12 for visualization purpose only.

fill-in ratio is often used to measure the efficiency of the factorization, it is interesting to note that in all point-block factorizations shown in the table, the fill-in ratio is reduced in comparison with the corresponding pointwise versions, even in the case of BLU. By changing LU to BLU, the compute time is reduced by almost 50% when the number of processors is not large. In the cases of $BILU(l)$, although there is a mild growth in the number of GMRES iterations, the compute time is further reduced. Comparing with the results using LU factorization, using $BILU(l)$ as the subdomain solve saves nearly 75% of the compute time when the number of processors is small, and saves over 20% of the compute time when the number of processors is large.

np	LU				BLU			
	NI	GMRES	time	fill-in	NI	GMRES	time	fill-in
64	2.0	33.25	218.26	22.84	2.0	33.25	133.47	19.71
128	2.0	39.25	65.21	20.13	2.0	39.25	43.52	14.47
256	2.0	44.25	23.53	14.47	2.0	44.25	16.66	11.35
512	2.0	52.55	10.16	10.38	2.0	52.55	7.56	8.35
1024	2.0	58.85	5.14	7.15	2.0	58.85	3.94	6.71
np	BILU(1)				BILU(2)			
	NI	GMRES	time	fill-in	NI	GMRES	time	fill-in
64	2.0	56.40	44.21	2.38	2.0	44.95	38.21	4.79
128	2.0	59.90	22.44	2.36	2.0	48.95	25.73	4.67
256	2.0	62.85	12.07	2.35	2.0	52.55	13.53	4.57
512	2.0	67.50	6.33	2.33	2.0	59.00	7.03	4.47
1024	2.0	71.40	3.06	2.29	2.0	63.35	4.39	4.59

Table 1: Performance with respect to the number of processors for different subdomain solvers. The tests are carried on a mesh with $1.25 \cdot 10^6$ unknowns with a fixed overlapping size $\delta = 1$. “ np ” denotes the number of processors. “NI” denotes the average number of Newton iterations per time step. “GMRES” denotes the average number of GMRES iterations per Newton step. “time” refers to the average compute time, in seconds, per time step. “fill-in” refers to the average fill-in ratio needed in the subdomain factorization per iteration.

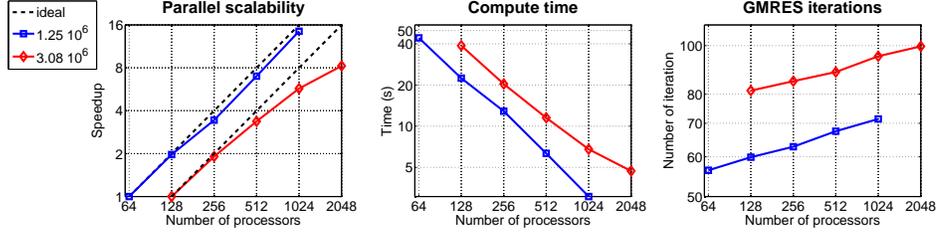


Figure 4: Parallel speedup, average compute time per time step, and average number of GMRES iterations per Newton iteration for the benchmark problem with increasing number of processors. The number of unknowns of each problem is listed in the legend. The tests are run with a fixed overlapping size $\delta = 1$ and BILU(1) is the subdomain solver.

4.2. A two-branch artery case

In this subsection, we perform simulations for a bifurcating artery with two branches that is part of the pulmonary artery of a patient. The arterial wall thickness is assume to be 10% of the local arterial diameter. For the inlet, we prescribe a pulsatile periodic flow wave, with a period T of 0.6 s. For the outlets, the relation $P = QR$ is implicitly prescribed on the outflow boundaries as the resistance boundary condition, where P is the fluid pressure and $Q = \int_{\Gamma} \mathbf{u}_f \cdot \mathbf{n} ds$ represents the flow rate at the outflow boundaries [16, 41]. The resistance $R = 1408.0 \text{ dyn} \cdot \text{s}/\text{cm}^5$ and $R = 677.6 \text{ dyn} \cdot \text{s}/\text{cm}^5$ at the left and the right artery outlet, respectively. The elastic arterial wall is characterized with density of $1.2 \text{ g}/\text{cm}^3$, Young's modulus of $1.5 \times 10^6 \text{ g}/(\text{cm s}^2)$, and the Poisson ratio of 0.48. As mentioned earlier in the paper, the external force from the surrounding tissues is modeled as a damping term added to the elasticity equation, and the coefficient of the term is chosen as $\alpha = 6.0 \times 10^3$, which is the same as what is used in the literature [33, 37]. The blood is modeled with a density of $1.0 \text{ g}/\text{cm}^3$ and viscosity of

0.035 $g/(cm\ s)$. The geometry and measured resistance values for this model come from clinical data, provided by University of Colorado Medical School. We initialize the Newton iteration by setting the initial wall velocity to zero and use the solution of the steady state FSI problem as the initial conditions for the unsteady problem. The simulations are run for 3 cardiac cycles with a time step size of 0.001 s. In Figure 5, we show the computed flow speed results and pressure at the inlet, the left artery outlet (LPA), and the right artery outlet (RPA) during one cardiac cycle. The outflow lags the inflow due to the compliance of the arterial wall. The computed phase shift between the inflow and the outflow at RPA is 0.02 s. Figure 6 shows two snapshots of the fluid velocity field at two phases of the cardiac cycle, the peak systole, and early-diastole. The fully three-dimensional flow field is quite complex, especially in the diastole phase. Figure 7 shows the arterial wall velocity vectors at the same two phases, illustrating the corresponding wall movement in response to the fluid dynamics. Such complex flow structures are usually very difficult to be measured clinically, high resolution computation provides a unique way to reveal the phenomena.

To investigate the parallel performance and scalability of our solver for this problem, we choose the same linear and nonlinear stopping criterions as in the previous benchmark tests. The time step size is fixed as $\Delta t = 0.001\ s$, and the simulation is stopped after 10 time steps. Figure 8 shows the strong scalability for solving the problem discretized on two meshes; one with $1.24 \cdot 10^6$ degrees of freedom, and the other with $4.61 \cdot 10^6$ degrees of freedom. For the small mesh, the strong scalability stays close to be linear until the number of processors becomes larger than 512. For the larger mesh,

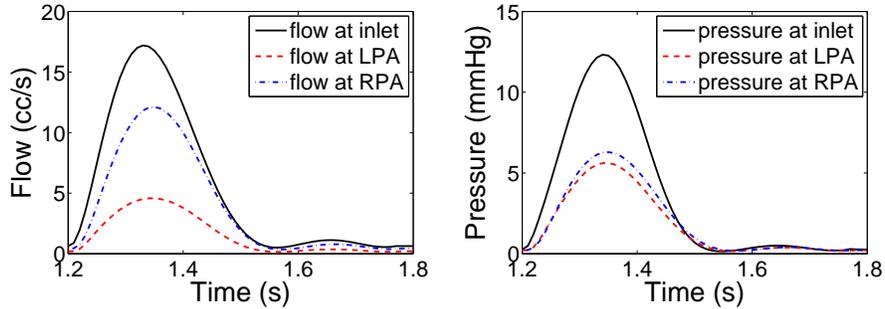


Figure 5: Flow and pressure at the inlet and outlets over one cardiac cycle for the two-branch artery model, obtained using the resistance outflow boundary condition. Figure on the left represents the flow rate at the inlet and outlets, and figure on the right shows the fluid pressure at the inlet and outlets. The test is carried on a mesh with $3.57 \cdot 10^6$ element and $4.61 \cdot 10^6$ degrees of freedom.

the strong scalability stays close to be linear until $np = 2048$. It is worth noting that the growth in the number of GMRES iterations for large processor counts may be a problem if we consider to solve the problem on a much larger mesh and with a larger number processors. In those situations, one possible solution to improve the scalability is to use of a multilevel method. In Table 2, we show the results with respect to different subdomain solvers. We should mention that GMRES fails to converge when using BILU(1) as the subdomain solver. But by increasing the fill-in level from 1 to 2 in the point-block incomplete factorization we are able to reduce the ill-conditioning effect and GMRES converges nicely.

4.3. Complex branching artery case

Next we conduct experiments for a larger and more complicated artery with many branches obtained from a biplane angiography image of the pul-

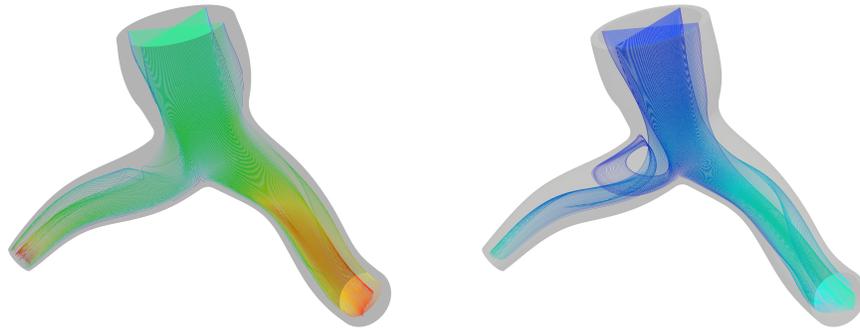


Figure 6: Flow in part of the pulmonary artery with two branches at the peak systole (left) and the early diastole (right). The fluid streamlines are colored by velocity magnitude.

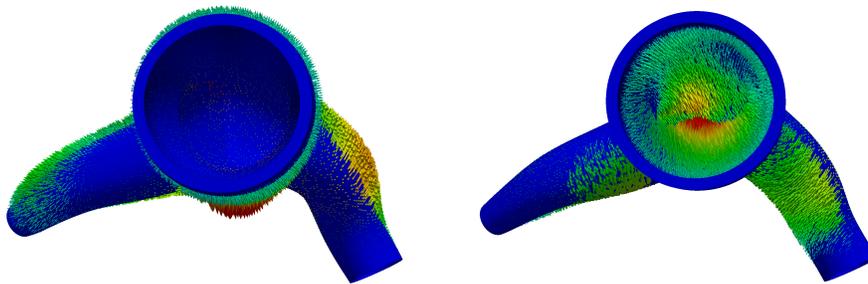


Figure 7: Arterial wall velocity vectors obtained at two points of the cardiac cycle: peak systole (left), early diastole (right).

np	LU				BLU			
	NI	GMRES	time	fill-in	NI	GMRES	time	fill-in
128	2.0	62.50	95.38	16.73	2.0	62.50	50.73	14.66
256	2.0	76.50	35.16	13.23	2.0	76.50	21.92	10.62
512	2.0	102.25	17.06	8.91	2.0	102.30	9.58	8.91
1024	2.0	129.45	8.09	6.57	2.0	129.45	6.18	5.10
np	BILU(2)				BILU(3)			
	NI	GMRES	time	fill-in	NI	GMRES	time	fill-in
128	2.0	110.30	22.21	4.76	2.0	71.85	25.43	8.11
256	2.0	118.75	12.87	4.58	2.0	83.50	14.93	7.87
512	2.0	127.15	7.53	4.75	2.0	111.75	9.08	7.62
1024	2.0	148.50	4.94	4.86	2.0	131.45	5.71	7.84

Table 2: Performance with respect to the number of processors for different subdomain solvers for the two-branch model. The tests are carried on a mesh with $1.24 \cdot 10^6$ unknowns with a fixed overlapping size $\delta = 1$. “ np ” denotes the number of processors. “NI” denotes the average number of Newton iterations per time step. “GMRES” denotes the average number of GMRES iterations per Newton step. “time” refers to the average compute time, in seconds, per time step. “fill-in” refers to the average fill-in needed in the factorization per iteration.

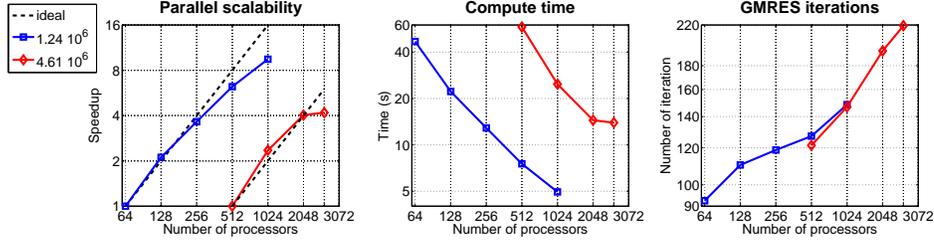


Figure 8: Parallel speedup, average compute time per time step, and average number of GMRES iterations per Newton iteration for the two branching problem with increasing number of processors. The number of unknowns of each mesh is listed in the legend. The tests are run with a fixed overlapping size $\delta = 1$.

monary artery of a patient. We assume the wall thickness is 10% of the arterial diameter. The arterial wall density is 1.2 g/cm^3 ; the Young’s modulus of the arterial wall is $7.5 \times 10^5 \text{ g/(cm s}^2)$; the Poisson ratio is 0.48. The fluid density is 1.0 g/cm^3 , and the viscosity is 0.035 g/(cm s) . For the inlet, we prescribe a pulsatile periodic flow with period of $T = 1.0 \text{ s}$, mapped to a parabolic velocity profile. The zero-traction boundary conditions are imposed at the outflows. Since the purpose of these simulations is mainly to test the performance of our algorithm, the choice of boundary conditions may not be physiological realistic, but are chosen from the literature [4, 5]. Simulation results for this branching model are shown in Figure 9.

In Figure 10, we report the parallel performance of our solution algorithm to the branching artery model. The simulations are performed on two different meshes, and the reported results the average values obtained from the first 10 and 100 time steps. Our algorithm again shows very good scalability, the parallel speedup is nearly linear as we increase the number of processors to 3072. For the additive Schwarz preconditioner, the overlapping parameter

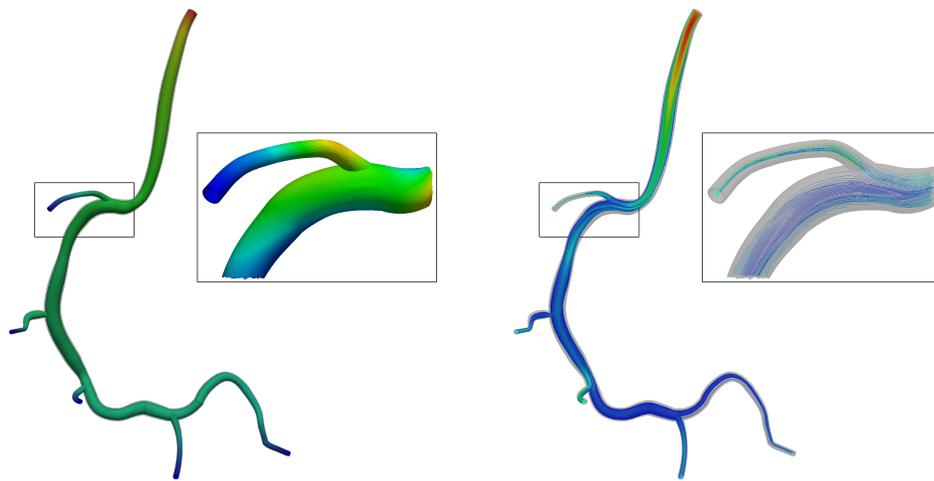


Figure 9: Results of the simulation of part of the pulmonary artery. In the large images, the fluid shaded by pressure is shown on the left, and the fluid velocity colored in its magnitude is shown on the right. The arterial wall is shown in a solid shade in both images. In the inset images, the arterial wall shaded by the norm of the displacement is shown on the left, and the fluid streamlines colored by vorticity is shown on the right.

δ is important for the fast convergence of GMRES. Note that the additive Schwarz preconditioner reduces to a block-Jacobi preconditioner when $\delta = 0$. In Table 3, we show the results with various choices of δ on different meshes and number of processors. By increasing δ , the average number of GMRES iterations decreases. However, smaller overlapping sizes (e.g., $\delta = 1$) produce better timing results. We also remark that larger δ helps in improving the robustness of the preconditioner. In some cases, the convergence of linear solver is difficult to achieve when $\delta = 0$.

Besides parallel performance and scalability, another important consideration in the design of discretization schemes and solution algorithms for the fluid-structure interaction problems is the robustness with respect to some of the important physical parameters, in particular, the fluid density and the wall density. It has been reported in some references that the convergence becomes more difficult to achieve if the density of the fluid and the arterial wall are close to each other [8], or if the fluid is much denser than the arterial wall [29]. Table 4 shows that our fully coupled solver performs quite well for a wide range of fluid density and arterial wall density in terms of the number of Newton iterations, the number of GMRES iterations, and the total compute time.

There are two important physical parameters in describing the properties of the arterial wall, the Young's modulus E which is related to the stiffness of the arterial wall and the Poisson ratio ν which represents the incompressibility of the arterial wall. The problems become harder to solve numerically as E becomes large and ν is closer to 0.5. In Table 5, our algorithm shows robust convergence with respect to both parameters.

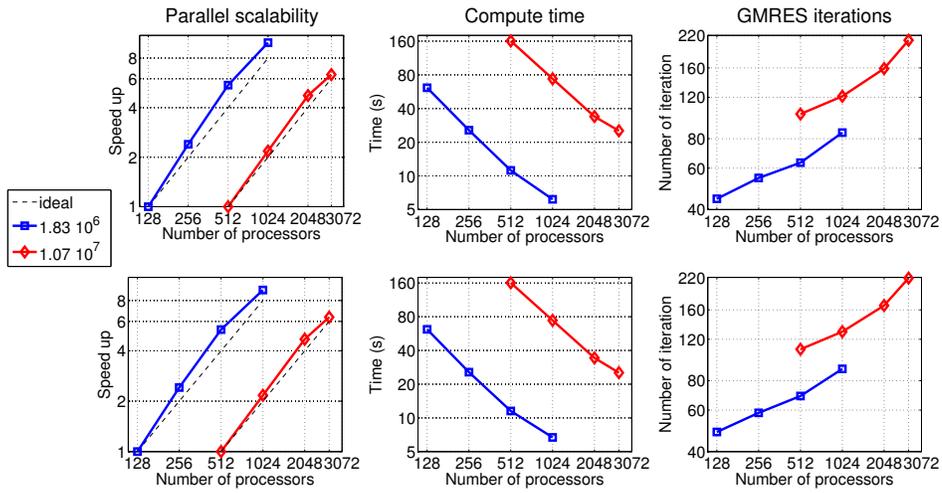


Figure 10: Parallel speedup, average compute time per time step, and average GMRES iterations per Newton iteration for the complex branching problem with increasing number of processors. The top 3 figures show the results obtained from the simulation of first 10 time steps, and the bottom three figures show the results obtained from the simulation of first 100 time steps. The number of unknowns of each problem is listed in the legend. The tests are run with a fixed overlapping size $\delta = 1$.

unknowns	np	overlap δ	Newton	GMRES	time
$1.83 \cdot 10^6$	512	0	2.0	104.75	16.15
$1.83 \cdot 10^6$	512	1	2.0	63.30	11.89
$1.83 \cdot 10^6$	512	2	2.0	55.80	13.06
$1.83 \cdot 10^6$	512	3	2.0	51.60	16.05
$1.83 \cdot 10^6$	1024	0	2.0	165.95	10.01
$1.83 \cdot 10^6$	1024	1	2.0	84.95	6.16
$1.83 \cdot 10^6$	1024	2	2.0	71.65	6.61
$1.83 \cdot 10^6$	1024	3	2.0	65.05	9.51
$1.07 \cdot 10^7$	512	0	2.0	260.85	249.65
$1.07 \cdot 10^7$	512	1	2.0	101.90	160.50
$1.07 \cdot 10^7$	512	2	2.0	74.15	197.05
$1.07 \cdot 10^7$	512	3	2.0	64.50	258.04
$1.07 \cdot 10^7$	1024	0	2.0	430.65	170.66
$1.07 \cdot 10^7$	1024	1	2.0	121.20	73.66
$1.07 \cdot 10^7$	1024	2	2.0	96.90	94.40
$1.07 \cdot 10^7$	1024	3	2.0	88.20	140.72
$1.07 \cdot 10^7$	2048	0	2.0	669.30	93.71
$1.07 \cdot 10^7$	2048	1	2.0	159.00	33.89
$1.07 \cdot 10^7$	2048	2	2.0	118.80	38.19
$1.07 \cdot 10^7$	2048	3	2.0	102.50	54.88

Table 3: The effect of various choices of the overlapping parameter δ on different mesh sizes and number of processors. “ np ” denotes the number of processors. “Newton” denotes the average Newton iteration per time step. “GMRES” denotes the average GMRES iterations per Newton step. “time” refers to the average compute time, in seconds, per time step.

ρ_f	ρ_s	Newton	GMRES	time (s)
0.01	1.0	2.0	231.15	9.95
0.1	1.0	2.0	142.65	8.28
1.0	1.2	2.0	85.300	6.164
10.0	1.0	2.1	137.571	8.594
100.0	1.0	3.0	99.267	11.132
1.0	0.01	2.0	87.550	8.809
1.0	0.1	2.0	87.400	9.1795
1.0	10.0	2.0	164.100	11.353
1.0	100.0	2.0	104.600	9.320

Table 4: Performance for different combinations of fluid density ρ_f and wall structure density ρ_s for the complex branching model. The dynamic viscosity ν_f is kept as $0.035 \text{ cm}^2/\text{s}$. The tests are run on a mesh with $1.83 \cdot 10^6$ degrees of freedom and 1024 processors.

E ($g/(cm\ s^2)$)	ν	Newton	fGMRES	time (s)
$7.5 \cdot 10^5$	0.45	2.0	74.30	5.84
$1.5 \cdot 10^6$	0.45	2.0	112.65	6.58
$3.8 \cdot 10^6$	0.45	2.0	166.70	7.58
$7.5 \cdot 10^6$	0.45	2.0	220.10	8.52
$7.5 \cdot 10^5$	0.45	2.0	74.30	5.84
$7.5 \cdot 10^5$	0.47	2.0	79.85	5.93
$7.5 \cdot 10^5$	0.48	2.0	84.95	6.02
$7.5 \cdot 10^5$	0.49	2.0	182.10	7.86

Table 5: Performance for various values of Young’s modulus E_s and Poisson ratio ν for the complex branching model. The tests are run on a mesh with $1.83 \cdot 10^6$ degrees of freedom and 1024 processors.

5. Conclusion

In this paper, we studied an ALE based general framework for fully implicit and fully coupled simulation of three-dimensional fluid-structure interaction problems. The investigation includes a finite element discretization with a time dependent stabilization on moving unstructured meshes, a scalable monolithic domain decomposition based Newton-Krylov-Schwarz method for solving the coupled system of nonlinear algebraic equations, and a software package runs on supercomputers with thousands of processors. As an example, we applied the technology to the simulation of blood flows in patient-specific arteries and demonstrated that the algorithm is both accurate and efficient. In particular, the algorithm and software show a great deal of robustness with respect to the complicated patient-specific geome-

tries, large meshes and large number of processors. Superlinear scalability was observed for problems with tens of millions of degrees of freedom and on a machine with more than three thousand processors. We plan to further extend the approach and the software framework to include multilevel capability, which is needed for supercomputer with larger processor counts and for large-scale simulations.

6. Acknowledgments

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