NKS for Fully Coupled Fluid-Structure Interaction with Application

Andrew T. Barker[1] and Xiao-Chuan Cai[2]

[1] Department of Applied Mathematics, University of Colorado, Boulder, CO 80309-0526, andrew.barker@colorado.edu
[2] Department of Computer Science, University of Colorado, Boulder, CO 80309-0430, cai@cs.colorado.edu

1 Introduction

Newton-Krylov-Schwarz algorithms have been used in many areas and are often quite scalable and robust. In this paper we explore the application of Schwarz type domain decomposition preconditioners to some fully coupled systems for fluid-structure interaction. In particular, we are interested in developing a scalable parallel framework for the simulation of blood flow in human arteries [11]. In [2, 3], coupled fluid-structure problems are solved in 3D for patient-specific artery models, with emphasis on accurately representing vessel geometry, on constitutive model for the artery walls, and other physical concerns. In this paper we focus on a class of parallel domain decomposition algorithms for solving the coupled systems and report on the robustness and parallel scalability of the algorithms.

Very often in the simulation of fluid-structure interaction, fluid and structure are iteratively coupled, as in [4, 5, 7]. That is, fluid and structure subproblems are solved alternately (or in parallel), passing boundary conditions between them, until the solutions are compatible at the fluid-structure interface, and then the simulation proceeds to the next time step. However, this approach often requires small timesteps, can become unstable, and can reduce the order of accuracy of the solution [8]. In contrast, we use fully monolithic coupling, where the fluid and the structure are solved together as one system.

2 Governing Equations

We use a linear elastic model for the structure. The primary variable in the structure equations is the displacement vector $\mathbf{x}_s$. Define σ_s as the stress-strain relation or Cauchy stress tensor

$$\sigma_s = \lambda_s(\nabla \cdot \mathbf{x}_s)I + 2\mu_s(\nabla \mathbf{x}_s + \nabla \mathbf{x}_s^T)$$

where λ_s and μ_s are the Lamé constants. The equilibrium equation for linear elasticity is

$$\rho_s \frac{\partial^2 \mathbf{x}_s}{\partial t^2} = \nabla \cdot \sigma_s + \mathbf{f}_s. \tag{1}$$

We fix the structure displacement $\mathbf{x}_s = 0$ on the dry, non-interaction boundary Γ_S; the boundary conditions on the fluid-structure interaction boundary Γ_w will be presented when we discuss the fluid-structure coupling.

The mesh points of our fluid domain move, and the displacements of the mesh nodes from their original reference configuration define a separate field that we need to represent. For the grid displacements $\mathbf{x}_f$, we simply use the Laplace equation

$$\Delta \mathbf{x}_f = 0 \tag{2}$$

in the interior of the domain, following [9]. In our numerical simulations this simple relation gives a smooth grid as the boundaries of the domain move, rarely causing problems with ill-conditioned elements. The boundary conditions for this field are either fixed zero Dirichlet conditions (at the inlet and outlet of the fluid domain) or are prescribed to follow the movement of the structure.

We model blood as a viscous incompressible Newtonian fluid, using the Navier-Stokes equations written in the ALE frame

$$\left.\frac{\partial \mathbf{u}_f}{\partial t}\right|_Y + [(\mathbf{u}_f - \omega_g) \cdot \nabla]\mathbf{u}_f + \frac{1}{\rho_f}\nabla p = \nu_f \Delta \mathbf{u}_f, \tag{3}$$

$$\nabla \cdot \mathbf{u}_f = 0. \tag{4}$$

Here $\mathbf{u}_f$ is the fluid velocity vector and p is the pressure. The given data include the fluid density ρ_f, and $\nu_f = \mu_f/\rho_f$, the kinematic viscosity. External body forces are ignored. Also, $\omega_g = \partial \mathbf{x}_f/\partial t$ is the velocity of the moving mesh in the ALE frame and the Y indicates that the time derivative is to be taken with respect to the ALE coordinates, not the Eulerian coordinates [9].

Boundary conditions for the fluid equations consist of a no-slip condition $\mathbf{u}_f = 0$ at rigid walls Γ_f, a Dirichlet condition where $\mathbf{u}_f$ takes a given profile at the inlet Γ_i, and a zero traction condition

$$\sigma_f \cdot \mathbf{n} = \mu_f(\nabla \mathbf{u}_f \cdot \mathbf{n}) - p\mathbf{n} = 0 \tag{5}$$

on the outlet Γ_o, where σ_f is the Cauchy stress tensor for the fluid and $\mathbf{n}$ is the unit outward normal.

At the fluid-structure interface we require that the structure velocity match the fluid velocity $\mathbf{u}_f = \partial \mathbf{x}_s/\partial t$ and we also enforce that the moving mesh must follow the solid movement $\mathbf{x}_f = \mathbf{x}_s$, so that the solid can maintain a Lagrangian description. The coupling of traction forces at the boundary can be written $\sigma_s \cdot \mathbf{n} = \sigma_f \cdot \mathbf{n}$ where $\mathbf{n}$ is the unit normal vector at the fluid-solid interface.

3 Spatial Discretization

Because of space constraints, we omit the full derivation of the weak form of the governing equations. We note two interesting points here. First, because of our moving grid, the variational spaces in which we seek a solution to the fluid subproblem are time-dependent. Second, the variational spaces associated with the fluid subproblem and the mesh subproblem depend implicitly on the current solution to the structure subproblem, as this solution provides essential boundary conditions for the fluid and mesh subproblems.

The spatial discretization is done with quadrilateral finite elements, with a conforming discretization at the fluid-structure interface, so that no special interpolation scheme is necessary to move information between fluid and structure.

We write the structure displacement vector $\mathbf{x}_s$ as $\mathbf{x}_s \approx \sum_j \varphi_j(x) x_j(t)$ and denote the vector of coefficients x_j as x_s. Using this approximation, we arrive at the semi-discrete system

$$M_s \frac{\partial^2 x_s}{\partial t^2} + C_s \frac{\partial x_s}{\partial t} + K_s x_s = F \tag{6}$$

where $C_s = \alpha M_s + \beta K_s$ is an added Rayleigh damping matrix where α and β are small parameters; typically $\alpha \approx 0.1$ and $\beta \approx 0.01$ [6].

We use biquadratic quadrilateral finite elements in our ALE discretization of the moving mesh. We approximate $\mathbf{x}_f \approx \sum_j \xi_j(x) x_j(t)$. This is a standard finite-element discretization of the Laplace equation resulting in $K_m x_f = 0$ with boundary conditions that depend on the structure subproblem.

The fluid is discretized with the LBB-stable $Q_2 - Q_1$ finite elements. Using finite-dimensional approximations $\mathbf{u}_f \approx \sum_j \varphi_j(x,t) u_j(t)$ and $p \approx \sum_j \psi_j(x,t) p_j(t)$ we can write the semi-discrete Navier-Stokes equations in the ALE frame as

$$M_f \frac{\partial u}{\partial t} + B(u)u + K_f u - Q^T p = M_f f, \tag{7}$$

$$Qu = 0 \tag{8}$$

where M_f is a mass matrix, $B(u)$ represents the nonlinear convective operator, K_f is the discrete Laplacian, and Q is the discrete divergence operator.

The mesh displacement continuity and velocity continuity conditions are enforced directly at each timestep; we replace rows of the matrix corresponding to these degrees of freedom with rows representing the equations $x_s = x_f$, and similarly for the velocity. We also need to discretize the traction force that the fluid exerts on the solid boundary, namely $\sigma_f \cdot \mathbf{n} = \mu_f(\nabla \mathbf{u}_f \cdot \mathbf{n}) - p\mathbf{n}$. The result has block matrix form

$$\sigma_f \cdot \mathbf{n} = \begin{pmatrix} A_{uu} & A_{uv} & A_{up} \\ A_{vu} & A_{vv} & A_{vp} \end{pmatrix} \begin{pmatrix} u_f \\ v_f \\ p \end{pmatrix} = \begin{pmatrix} A_u & A_p \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix}. \tag{9}$$

This will be inserted as a force in the discrete form of the structure equations to enforce the traction matching condition at the fluid-structure interface.

4 Temporal Discretization

We use the trapezoid rule $y^{n+1} = y^n + (\Delta t/2)\left(f^{n+1} + f^n\right)$ which is a second-order accurate implicit scheme for all our time discretization.

For the structure time-stepping, we follow [6] in implementing the trapezoid rule by reducing the order of (6) from second order to first order. Our new vector of unknowns includes both solid displacement and velocity, $y = (x_s, \partial x_s/\partial t)^T$. Then

$$\frac{\partial y}{\partial t} = f(y,t) = \begin{pmatrix} \dfrac{\partial x_s}{\partial t} \\ M^{-1}(F(t) - K_s x_s - C_s \dfrac{\partial x_s}{\partial t}) \end{pmatrix}.$$

The trapezoid rule for this differential algebraic equation can be written

$$My^{n+1} = My^n + \frac{\Delta t}{2}\left[Ky^{n+1} + Ky^n + F^{n+1} + F^n\right]$$

where

$$M = \begin{pmatrix} I & \\ & M_s \end{pmatrix}, \quad K = \begin{pmatrix} & I \\ -K_s & -C_s \end{pmatrix}.$$

The moving mesh, like the continuity equation for the fluid, is enforced independent of time. So we simply require

$$K_m x_f^{n+1} = 0$$

at each time step.

Rescaling pressure by the timestep Δt, we apply a slightly modified version of the trapezoid rule to (7) to get

$$Mu^{n+1} = Mu^n + \frac{1}{2}\left[(S + \Delta t R^{n+1})u^{n+1} + (S + \Delta t R^n)u^n\right]$$

where

$$M = \begin{pmatrix} M_f & 0 \\ 0 & 0 \end{pmatrix}, \quad R^n = \begin{pmatrix} -B(u^n) - K_f & 0 \\ 0 & 0 \end{pmatrix}, \quad S = \begin{pmatrix} 0 & -Q^T \\ Q & 0 \end{pmatrix}.$$

We use the same time-stepping scheme for fluid and structure, so we can simply put the discretized fluid and structure problems together in one system with coupling enforced implicitly. In summary, we have

$$(M + W)y^{n+1} - My^n - \frac{\Delta t}{2}(Ky^{n+1} + Ky^n) - \frac{\Delta t}{2}(F^{n+1} + F^n) = 0 \qquad (10)$$

where

$$y^n = \begin{pmatrix} u^n \\ \Delta t\, p^n \\ x_f^n \\ x_s^n \\ \dot{x_s}^n \end{pmatrix}, \quad M = \begin{pmatrix} M_f & & \\ & I & \\ & & M_s \end{pmatrix},$$

$$W = \begin{pmatrix} & & \\ & K_m & \\ A_u & A_p & \\ & & \end{pmatrix}, \quad K = \begin{pmatrix} -B - K_f & -(1/\Delta t)Q^T & & \\ (1/\Delta t)Q & & & \\ & & & I \\ & & -K_s & -C_s \end{pmatrix}.$$

Though written in matrix form, many of the operators above are nonlinear. In particular the B term depends on u_f, and the K_f, M_f and Q terms depend on the moving mesh x_f. This implies that we have a Jacobian of the form

$$J = \begin{pmatrix} J_f & -Q^T & Z_m & & \\ Q & & Z_c & & \\ & & K_m & & \\ A_u & A_p & & I & -(\Delta t/2)I \\ & & & (\Delta t/2)K_s & M_s + (\Delta t/2)C_s \end{pmatrix} \tag{11}$$

where J_f is the Jacobian of the nonlinear term in the momentum equation and Z_m and Z_c are the nonlinear contributions of the moving mesh to the momentum and continuity equations. The form of Z_m and Z_c are unknown, and our implementation of the Jacobian simply ignores them, which is a reasonable approximation as long as the mesh movement is slow, i.e., the timestep is sufficiently small.

5 Solving the Nonlinear System

At each timestep, we solve the nonlinear system (10) with an inexact Newton method with line search. At each Newton step we solve a preconditioned linear system of the form $J(y)M^{-1}(Ms) = z$ for the Newton correction s, where M^{-1} is a one-level additive Schwarz preconditioner [10, 12, 13]. In this domain decomposition preconditioner, the formation of subdomains does not consider the fluid-structure boundary, so that a subdomain may contain fluid elements, structure elements, or both. Subdomain solves are done by LU factorization with homogeneous Dirichlet boundary conditions on the boundaries for all solution variables, including the fluid pressure.

In practice, we order the unknowns for the Jacobian system not by field ordering as in (11), but by element ordering. The choice of ordering can have significant effect on the convergence properties of the solver. By this choice, the nonzero-block structure is banded. That is, within each element the unknowns are ordered as in (11), but globally the matrix looks like the nine-point stencil for a Poisson equation.

6 Numerical Results

Our solver is implemented using PETSc [1]. All computations are performed on an IBM BlueGene/L supercomputer at the National Center for Atmospheric Research with 1024 compute nodes.

We begin all our simulations with zero initial conditions for structure displacement and fluid velocity, therefore compatibility between fluid and structure is easily satisfied in the initial conditions. In all the numerical results in this paper, we use a timestep $\Delta t = 0.01$, a Young's modulus $E = 1.0 \cdot 10^5$, we stop the linear solver when the preconditioned residual has decreased by a factor of 10^{-4} and we stop the Newton iteration when the nonlinear residual has decreased by a factor of 10^{-6}. We set GMRES to restart every 40 iterations, and have the structural damping parameters $\alpha = 0.1, \beta = 0.01$. Simulations begin with zero initial conditions and proceed 10 timesteps, reporting average walltime and nonlinear iteration count per timestep, and average GMRES iterations per Newton step.

Our fluid-structure interaction simulations can deal with large deformations of the computational grid without the quality of the mesh degrading and without affecting convergence, and we maintain sufficient spatial resolution to resolve vortices and other interesting flow features.

The scalability of our algorithm is presented in Table 1. Our method scales well with respect to number of processors and scales fairly well with respect to problem size. It is also worth noting the large grid sizes and processor counts that we have used with success. The growth in GMRES iterations for large processor counts suggests that the less than perfect speedup could probably be improved by use of a multilevel preconditioner.

unknowns	np	GMRES	Newton	time
$1.0 \cdot 10^6$	64	9.3	5.0	123.44
	128	13.4	5.0	57.11
	256	18.2	5.0	36.41
	512	24.0	5.0	22.08
$2.1 \cdot 10^6$	128	17.5	4.8	125.31
	256	21.5	4.8	66.11
	512	29.7	4.8	39.97
	1024	35.9	4.8	22.90
	2048	40.0	4.8	17.25
$2.6 \cdot 10^6$	128	15.1	4.7	198.34
	256	20.1	4.7	100.23
	512	29.3	4.7	46.50
	1024	40.0	4.7	28.11
	2048	48.6	4.7	21.10

Table 1. Speedup and scalability. In this table ASM overlap $\delta = 2$, Reynolds number = 132.02, $\nu_s = 0.30$

Our simulation is also robust with respect to physical parameters. In Table 2a, we show numerical results for various Reynolds numbers. Many blood flow simulations, for example [2], use Reynolds numbers in the range 30–100, but we can exceed that without much difficulty. As the Poisson ratio ν_s approaches $1/2$ the structure becomes incompressible and the structure problem becomes more numerically challenging; our solver is fairly robust also in this respect (results not shown). In some FSI methods, the case where fluid and structure densities are nearly equal is particularly difficult. Our monolithic coupling avoids this difficulty, see Table 2b.

ρ_s	ρ_f	GMRES	Newton
10^{-6}	10^{-6}	57.8	2.5
10^{-6}	10^{-3}	41.1	3.8
10^{-6}	1.0	7.3	5.6
10^{-6}	10.0	5.8	7.9
1.0	10^{-6}	59.0	2.3
1.0	10^{-3}	40.5	3.7
1.0	1.0	7.5	5.4
1.0	10.0	5.8	7.9
10^6	10^{-6}	60.4	2.4
10^6	10^{-3}	64.7	2.3
10^6	1.0	24.6	4.0
10^6	10.0	11.0	4.2

unknowns	Re	GMRES	Newton
	33.00	12.0	4.8
	66.01	12.1	4.8
$2.1 \cdot 10^6$	132.02	12.2	4.8
	264.03	12.5	4.8
	1056.12	12.7	10.0
	33.00	12.9	4.7
	66.01	13.1	4.7
$2.6 \cdot 10^6$	132.02	13.5	4.7
	264.03	13.5	4.7
	1056.12	13.7	9.9

Table 2. (a) Sensitivity of algorithm to various fluid densities (ρ_f) and solid densities (ρ_s); these problems have $6.5 \cdot 10^5$ unknowns and tests are done with 128 processors. (b) Sensitivity to Reynolds number with 256 processors. In both (a) and (b) ASM overlap $\delta = 8$ and $\nu_s = 0.30$

7 Conclusion

Accurate modeling of blood flow in compliant arteries is a computational challenge. In order to meet this challenge, we need not only to model the physics accurately but also to develop scalable algorithms for parallel computing. In this paper we develop a Newton-Krylov-Schwarz solver that scales well in parallel and is effective for solving the implicitly coupled fluid-structure interaction problem. Our method is quite robust with respect to different vessel geometries, Reynolds numbers, Poisson ratios, densities, spatial mesh sizes and time step sizes.

Acknowledgement. We thank K. Hunter, C. Lanning, R. Shandas, A. Quarteroni, F. Hwang, J. Wilson, and X. Yue for their help and suggestions in the project. The research was supported in part by DOE under DE-FC02-01ER25479 and DE-FC02-04ER25595, and in part by NSF under grants ACI-0305666, CNS-0420873, CCF-0634894, and CNS-0722023.

References

[1] Balay, S., Buschelman, K., Eijkhout, V., Gropp, W., Kaushik, D., Knepley, M., McInnes, L., Smith, B., Zhang, H.: PETSc users manual. Technical Report ANL-95/11 - Revision 2.1.5, Argonne National Laboratory, 2004.

[2] Bazilevs, Y., Calo, V.M., Zhang, Y., Hughes, T.J.R.: Isogeometric fluid-structure interaction analysis with applications to arterial blood flow. *Comput. Mech.*, 38:310–322, 2006.

[3] Figueroa, C., Vignon-Clementel, I., Jansen, K., Hughes, T., Taylor, C.: A coupled momentum method for modeling blood flow in three-dimensional deformable arteries. *Comput. Methods Appl. Mech. Engrg.*, 195:5685–5706, 2006.

[4] Formaggia, L., Gerbeau, J.F., Nobile, F., Quarteroni, A.: On the coupling of 3D and 1D Navier-Stokes equations for flow problems in compliant vessels. *Comput. Methods Appl. Mech. Engrg.*, 191:561–582, 2001.

[5] Formaggia, L., Gerbeau, J.F., Nobile, F., Quarteroni, A.: Numerical treatment of defective boundary conditions for the Navier-Stokes equations. *SIAM J. Numer. Anal.*, 40:376–501, 2002.

[6] Hughes, T.: The Finite Element Method: Linear Static and Dynamic Finite Element Analysis. Dover, 2000.

[7] Hunter, K., Lanning, C., Chen, S., Zhang, Y., Garg, R., Ivy, D., Shandas, R.: Simulations of congenital septal defect closure and reactivity testing in patient-specific models of the pediatric pulmonary vasculature: a 3D numerical study with fluid-structure interaction. *J. Biomech. Eng.*, 128(4): 564–572, 2006.

[8] E. Kuhl, S. Hulshoff, and R. de Borst. An arbitrary Lagrangian Eulerian finite-element approach for fluid-structure interaction phenomena. *Internat. J. Numer. Methods Engrg.*, 57:117–142, 2003.

[9] Nobile, F.: Numerical Approximation of Fluid-Structure Interaction Problems with Application to Haemodynamics. PhD thesis, École Polytechnique Fédérale de Lausanne, 2001.

[10] Ovtchinnikov, S., Dobrian, F., Cai, X.-C., Keyes, D.E.: Additive Schwarz-based fully coupled implicit methods for resistive Hall magnetohydrodynamic problems. *J. Comput. Phys.*, 225(2):1919–1936, 2007. ISSN 0021-9991.

[11] Quarteroni, A., Tuveri, M., Veneziani, A.: Computational vascular fluid dynamics: problems, models and methods. *Comput. Vis. Sci.*, 2:163–197, 2000.

[12] Quarteroni, A., Valli, A.: Domain Decomposition Methods for Partial Differential Equations. Oxford University Press, Oxford, 1999.

[13] Toselli, A., Widlund, O.: Domain Decomposition Methods—Algorithms and Theory. Springer, Berlin, 2005.