

Centerline-Based Partition of Unity Coarse Space for Hemodynamic Simulations

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1 Introduction

The fully implicit numerical simulations of the unsteady incompressible Navier-Stokes equations often require solving a family of saddle-point systems with variable matrices due to the nonlinear convection term [1], one for each time step/Newton iteration. With suitable boundary conditions, this model is typically used to simulate the hemodynamic behavior in three-dimensional patient-specific arteries, enabling the prediction and assessment of the risk status of individual arteries [10]. Considering the large-scale and sparse structure of these saddle-point systems, we adopt a Krylov-Schwarz algorithm to solve them. The crucial part of this algorithm is the construction of an efficient Schwarz preconditioner, which often relies on a global coarse preconditioner [14]. The performance improvement of the coarse preconditioner is significant in reducing the computational time and cost.

For an unstructured mesh of complex arterial geometries, a suitable coarse mesh is typically non-nested and non-geometry-preserving in the construction of the Lagrangian coarse preconditioner, which brings challenges in the computation of restriction and extension matrices [2]. Partition of unity methods employ an element-based aggregation strategy to generate a nonoverlapping partition [14]. This method avoids the generation of a coarse mesh and the computation of low-frequency spectral components [13, 9, 7]. Each macro-element in the method consists of adjacent elements from the fine mesh. The coarse basis functions are defined as a family of finite element functions satisfying the partition of unity in the corresponding nonoverlapping partition. A simple class of functions is the finite element interpola-

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tion functions of characteristic functions. Its effectiveness is demonstrated in elliptic problems with quasi-homogeneous coefficients [12, 4]. For a moderate number of subdomains, the nonoverlapping subdomains generated in the one-level Schwarz method are usually used as the macro-elements in the partition of unity method. For massive subdomains, a general macro-element partition strategy is considered [3]. Such a partition of unity coarse space based on the existing subdomains can be directly applied in hemodynamic simulations, which significantly improves the convergence performance of Krylov subspace iterations compared with the one-level Schwarz method [11]. Some numerical results indicate that the macro-element partition has a crucial impact on the performance of the resulting partition of unity coarse space. Consequently, a suitable macro-element partition can further reduce both the dimension of the coarse space and the number of linear iterations.

In this paper, in the framework of the partition of unity coarse space, we introduce a centerline-based method to obtain the macro-element partition, referred to as the centerline-based partition of unity coarse space. We first obtain the centerline of an artery, and then generate a suitable coarse central-line mesh. The artery is subsequently divided into nonoverlapping subsegments based on the cross-sections associated with these coarse central-line mesh points. Such a centerline-based partition is easy to construct and implement and the resulting coarse space is usually low-dimensional. More importantly, leveraging the characteristics of geometry and blood flow, it efficiently improves the convergence performance of the Krylov-Schwarz solver compared with the partition from the existing one-level Schwarz method. Numerical experiments for a patient-specific artery show the scalability and effectiveness of the proposed coarse space.

2 Model problem and its discretization

Consider the unsteady incompressible Navier-Stokes equations in $\Omega \subset \mathbb{R}^3$

$$\begin{cases} \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) - \mu \Delta \mathbf{u} + \nabla p = \mathbf{0} & \text{in } \Omega \times (0, T), \\ \nabla \cdot \mathbf{u} = 0 & \text{in } \Omega \times (0, T), \\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{0} & \text{in } \Omega \times \{0\}, \end{cases} \quad (1)$$

where \mathbf{u} and p are the velocity and pressure, respectively. To describe the dynamic behavior of blood flow in a cardiac cycle T in a patient-specific artery, we consider an arterial computational domain Ω , and its boundary $\partial\Omega$ consists of the inlet Γ_I , the wall Γ_W and the multiple outlets $\Gamma_O = \cup_{i=1}^m \Gamma_O^i$. On the inlet and wall, we apply velocity Dirichlet and no-slip boundary conditions, respectively, i.e.,

$$\begin{aligned} \mathbf{u} &= \mathbf{u}_I(t) & \text{on } \Gamma_I, \\ \mathbf{u} &= \mathbf{0} & \text{on } \Gamma_W. \end{aligned} \quad (2)$$

where \mathbf{u}_i is a given inlet velocity. On the outlets, implicit resistive boundary conditions are adopted to approximate the behavior of the downstream vascular networks, described by

$$\mu \nabla \mathbf{u} \mathbf{n} - p \mathbf{n} = -R_i Q_i \mathbf{n} \text{ on } \Gamma_O^i, i = 1, \dots, m \quad (3)$$

R_i is a resistance parameter and $Q_i = \int_{\Gamma_O^i} \mathbf{u} \cdot \mathbf{n} d\Gamma_O^i$ is the unknown fluid flux on the outlet Γ_O^i with the unit outward normal vector \mathbf{n} . The boundary conditions (3) are weakly implemented, corresponding to the term $R_i Q_i \int_{\Gamma_O^i} \mathbf{v} \cdot \mathbf{n}$, in the corresponding weak formulation to ensure the well-posedness [8, 5].

For this problem, we employ a stabilized P1-P1 finite element method [6] and backward differentiation formulas (BDF) with a fixed time step size Δt for discretization on a shape-regular unstructured mesh \mathcal{T}_h , which results in a sequence of nonlinear systems [11]

$$F^n(X^n) = 0, n = 1, \dots, M, \quad (4)$$

where M is the number of time steps. The time integration is performed with the first-order BDF scheme for the first step and the second-order BDF for the remaining steps.

To solve these nonlinear systems, an inexact Newton algorithm with the previous numerical solution as the initial guess is implemented. The major challenge and computational cost arise from the solution of the linearized Jacobian systems due to the incompressibility constraint and the complexity of the geometry. Considering that these Jacobian matrices are sparse but indefinite, we use a Krylov-Schwarz method to solve these linear systems. The effectiveness of this method is determined by the Schwarz preconditioner. We now introduce a simple and efficient two-level additive Schwarz preconditioner.

In the context of overlapping Schwarz methods, we first carry out a domain decomposition for Ω to generate np nonoverlapping subdomains $\{\Omega_i^0\}_{i=1}^{np}$, ensuring the consistency with \mathcal{T}_h , and then extend them to form an overlapping partition. Specifically, the overlapping subdomain Ω_i^δ with an overlap layer δ is obtained by the layer-wise method

$$\Omega_i^{k+1} = \Omega_i^k \cup \{K \in \mathcal{T}_h \mid \partial K \cap \partial \Omega_i^{\delta-1} \neq \emptyset\}, \quad k = 0, \dots, \delta - 1. \quad (5)$$

Based on these nonoverlapping and overlapping subdomains, we define the corresponding subdomain restriction matrices R_i^0 and R_i^δ , respectively. In the implementation, the restriction matrix R_i^0 (or R_i^δ) operates on a global vector by selecting only those entries corresponding to degrees of freedom in Ω_i^0 (or Ω_i^δ , respectively). Furthermore, let R_0 denote a coarse restriction matrix, and its rows form a discrete coarse space. Then, the two-level overlapping restricted additive Schwarz preconditioner for a Jacobian matrix J is defined as follows

$$P_{2s}^{-1} = \sum_{i=1}^{np} \left(R_i^0 \right)^T J_i^{-1} R_i^\delta + R_0^T J_0^{-1} R_0 := P_{1s}^{-1} + P_c^{-1}, \quad (6)$$

where $J_i = R_i^\delta J (R_i^\delta)^T$, $i = 1, \dots, np$ are the overlapping subdomain Jacobian matrices and $J_0 = R_0 J (R_0)^T$ represents a coarse matrix from the projection of J onto the coarse space. In the next section, we focus on the construction of the coarse space and the corresponding restriction matrix R_0 using partition of unity functions.

3 Centerline-based partition of unity coarse space

In this section, we introduce a centerline-based partition of unity coarse space. In the context of finite element spatial discretization, we focus on the coarse basis functions, which are in the finite element space V_h . We first review the definition of partition of unity functions in a general scalar finite element space V_h .

Definition 1 A family of finite element functions $\{\varphi_0^i\}_{i=1}^{N_0} \in V_h$ is a partition of unity if it satisfies the following conditions

$$\sum_{i=1}^{N_0} \varphi_0^i = 1, \quad \text{and } 0 \leq \varphi_0^i \leq 1, i = 1, \dots, N_0. \quad (7)$$

Let $\{\varphi_0^i\}_{i=1}^{N_0}$ be a family of partition of unity finite element functions. Then the corresponding partition of unity coarse space is defined as

$$V_0 = \text{span} \left\{ \varphi_0^1, \dots, \varphi_0^{N_0} \right\}, \quad (8)$$

which is a subspace of V_h . To determine the partition of unity functions, a commonly used method is to adopt locally supported functions based on a nonoverlapping or overlapping partition of the computational domain Ω [14]. For simplicity, in the construction of partition of unity functions, we focus on the nonoverlapping partition with the subregions denoted by $\{S_i\}_{i=1}^{N_0}$, which are matched with the fine mesh \mathcal{T}_h with mesh points $\{\mathbf{x}^j\}_{j=1}^N$, where N is the number of fine mesh points. Then we define the finite element functions φ_0^i by

$$\varphi_0^i(\mathbf{x}^j) = \begin{cases} 1, & \mathbf{x}^j \in S_i \\ 0, & \text{otherwise} \end{cases} \quad i = 1, \dots, N_0. \quad (9)$$

which satisfy the conditions (7) and actually indicate the special values of the coarse basis functions at the fine mesh points. The restriction operator $\mathcal{R}_0^s : V_h \rightarrow V_0$ projects a finite element function in V_h into the subspace V_0 . The corresponding restriction matrix $R_0^s = (\varphi_0^i(\mathbf{x}^j))$ is an N_0 by N sparse matrix with N nonzero values.

For the blood flow problem (1)–(3), it includes three velocity components and one pressure component. Consequently, we define a partition of unity vector finite element coarse space by

$$\mathbf{V}_0 = [V_0]^4 := V_0 \oplus V_0 \oplus V_0 \oplus V_0. \quad (10)$$

In this case, the restriction matrix is the block diagonal matrix

$$R_0 = \text{diag}(R_0^s, R_0^s, R_0^s, R_0^s). \quad (11)$$

We now introduce the centerline-based nonoverlapping partition. For the centerline Ω_{cl} of Ω , we generate a suitable coarse mesh \mathcal{T}_h^{cl} . For all central-line mesh points $\{\mathbf{x}_{cl}^i\}_{i=1}^{N_{cl}}$, we compute corresponding unit tangential vectors $\{\boldsymbol{\tau}_{cl}^i\}_{i=1}^{N_{cl}}$. Let $\{(\mathbf{x}_{cl}^{e_1}, \mathbf{x}_{cl}^{e_2})\}_{i=1}^{N_{cl}^e}$ be the edge segments. For simplicity, we assume that there are N_{cl}^b bifurcations, and each bifurcation includes one parental inlet $\mathbf{x}_{cl}^{b_1}$ and two outlets $\mathbf{x}_{cl}^{b_2}, \mathbf{x}_{cl}^{b_3}$, denoted as $(\mathbf{x}_{cl}^{b_1}, \mathbf{x}_{cl}^{b_2}, \mathbf{x}_{cl}^{b_3})$. For each mesh point \mathbf{x}_{cl}^i , we define the corresponding cross-section by $C_s^i = \{\mathbf{x} \in \Omega \mid \mathbf{x} - \mathbf{x}_{cl}^i \perp \boldsymbol{\tau}_{cl}^i\}$, $i = 1, \dots, N_{cl}$. Use these cross-sections, the artery Ω can be divided into N_0 nonoverlapping subdomains $\{S_i\}_{i=1}^{N_0}$,

$$S_i = \begin{cases} S_i^e, & i = 1, \dots, N_{cl}^e \\ S_{i-N_{cl}^e}^b, & i = N_{cl}^e + 1, \dots, N_0 \end{cases} \quad (12)$$

where $N_0 = N_{cl}^e + N_{cl}^b$, and

$$S_i^e = \{\mathbf{x} \in \Omega \mid \mathbf{x} \text{ is enclosed by } C_s^{e_1}, C_s^{e_2}, \text{ and } \Gamma_W\}, \quad i = 1, \dots, N_{cl}^e, \quad (13)$$

$$S_j^b = \{\mathbf{x} \in \Omega \mid \mathbf{x} \text{ is enclosed by } C_s^{b_1}, C_s^{b_2}, C_s^{b_3}, \text{ and } \Gamma_W\}, \quad j = 1, \dots, N_{cl}^b. \quad (14)$$

The centerline-based partition reflects the primary behavior of blood flow from the inlet to the outlets along the centerline. In the implementation, a modified nonoverlapping partition is obtained to ensure that each subdomain consists of elements in \mathcal{T}_h .

4 Numerical experiments

In this section, we present some numerical experiments to illustrate the performance of the centerline-based partition of unity coarse preconditioner in a patient-specific artery, shown in Fig. 1. An unstructured mesh with over 8 million mesh elements and the fixed time step size $\Delta t = 0.01\text{s}$ are used for a spatial stabilized P1-P1 finite element discretization [11] and temporal BDF discretizations. The resulting nonlinear systems are solved by the inexact Newton method with the proposed two-level Schwarz preconditioned GMRES method. In the following simulations, we set blood density $\rho = 1.06\text{g/cm}^3$, viscosity $\mu = 0.035\text{g/(cm}\cdot\text{s)}$, and the cardiac cycle $T = 1\text{s}$. The inflow pulsatile velocity in a cardiac cycle is shown in Fig. 1. For the configuration of the algorithm, we set the absolute and relative tolerances $a_{\text{tol}} = 10^{-6}$

and $r_{\text{tol}} = 10^{-4}$, respectively. For the Schwarz method, the overlap parameter $\delta = 1$ is used to obtain the overlapping domain decomposition, and subproblems are solved by the incomplete LU factorization (ILU). For the centerline, three coarse meshes with 317, 361, and 522 mesh points are applied for the proposed centerline-based method, as illustrated in Fig. 1.

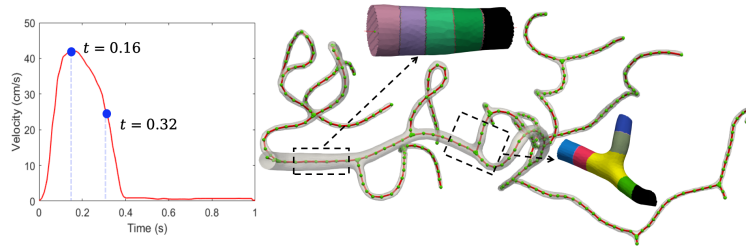


Fig. 1 A patient-specific inflow pulsatile velocity curve and artery with its centerline, where a coarse central-line mesh is used to generate a centerline-based nonoverlapping partition

In Fig. 2, we first show the performance of the one-level additive Schwarz preconditioner. The GMRES residuals decrease rapidly in the initial iterations and then slow down gradually. Such a phenomenon is often observed numerically due to the lack of global information exchange.

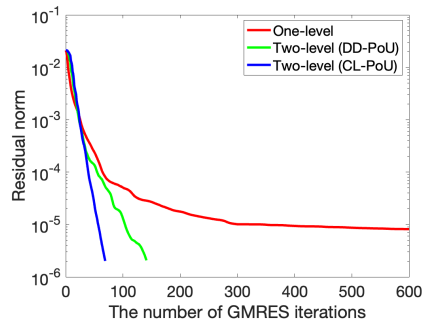


Fig. 2 Residual curve of the one-level and two-level Schwarz preconditioned GMRES iterations at the first Newton step at the peak systole $t = 0.16$ s.

We further study the effectiveness of the proposed two-level Schwarz preconditioner and compare the performance of partition of unity coarse preconditioners with the existing nonoverlapping partition (DD-PoU) and the centerline-based decomposition (CL-PoU), where the term “DD” in “DD-PoU” indicates that the partition comes from the underlying domain decomposition for the Schwarz method. The only difference between DD-PoU and CL-PoU is the construction of the nonoverlapping partition for the partition of unity. Fig. 2 also illustrates the effectiveness of

two-level methods, compared with the one-level method. The numbers of Newton and GMRES iterations are shown for different numbers of subdomains, fill-in levels of ILU factorization, and phases in a cardiac cycle in Table 1. An increase in the number of subdomains np results in a higher-dimensional DD-PoU coarse space, consequently yielding an obvious decrease in GMRES iterations. For the CL-PoU method, the coarse space dimension is independent of np , therefore the number of iterations remains nearly constant. Moreover, we also observe that the number of GMRES iterations of the CL-PoU method changes slightly with different central-line meshes. Compared with the DD-PoU method, the proposed CL-PoU method significantly improves the convergence performance of the GMRES method, while requiring an extremely low-dimensional coarse space, which implies a negligible computational cost in solving the coarse problem. These results demonstrate the effectiveness of the CL-PoU method in the construction of locally supported coarse basis functions.

Table 1 The numbers of Newton and GMRES iterations for the two-level preconditioner with partition of unity coarse spaces. DD-PoU and CL-PoU correspond to the nonoverlapping partitions from the existing domain decomposition and the proposed centerline-based decomposition, respectively. “ILU” represents the fill-in level of ILU, np denotes the number of subdomains, “Dim” is the dimension of coarse spaces, “Newton” represents the number of Newton iterations at the corresponding time step, and “GMRES” means the average number of GMRES iterations per Newton step.

$t(s)$	ILU	np	Newton	Two-level (DD-PoU)		Two-level (CL-PoU)					
				Dim	GMRES	Dim	GMRES	Dim	GMRES	Dim	GMRES
0.16	0	256		1024	185.00		78.50		79.00		80.00
		512	2	2048	133.50	1176	79.00	1432	77.00	1996	78.50
		1024		4096	112.50		79.50		76.50		78.50
	1	256		1024	137.50		55.00		56.00		58.00
		512	2	2048	99.00	1176	54.00	1432	54.50	1996	57.50
		1024		4096	84.00		54.50		54.50		58.00
0.32	0	256		1024	238.00		92.00		87.50		80.00
		512	2	2048	171.00	1176	89.50	1432	86.50	1996	79.00
		1024		4096	145.00		89.50		86.50		79.00
	1	256		1024	183.00		69.00		65.00		58.50
		512	2	2048	132.50	1176	66.50	1432	63.50	1996	58.50
		1024		4096	110.50		66.50		63.50		58.50

5 Conclusion

We introduce a centerline-based partition of unity coarse preconditioner to improve the performance of the two-level Schwarz preconditioner in the Newton-Krylov-

Schwarz framework for hemodynamic simulations. The coarse space consists of the partition of unity coarse basis functions, which are locally supported, obtained by the proposed central-line nonoverlapping partition. Such a coarse space is typically low-dimensional and easily implemented for unstructured meshes in complex computational domains. Compared with the existing nonoverlapping partition from the Schwarz method, the central-line partition leverages the arterial structure and provides a significant improvement in terms of the linear iteration, as observed in numerical results for patient-specific arteries. Future work includes a parallel implementation to evaluate its efficiency and scalability.

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