Scalable physics-guided data-driven component model reduction for Stokes flow

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Abstract

Stokes flow in repeated unit cell structures is extensively studied in applications for many natural and engineering processes. However, for large numbers of cells, resolving all scales can be prohibitively expensive using traditional numerical methods. To make the problem tractable, these methods often rely on volume-averaged approximations, resulting in accuracy issues. To address this, we propose a novel data-driven component model reduction approach that is constrained by the first-principle physics equation. This method employs reduced order modeling (ROM) to identify crucial physics modes in small-scale unit components and projects them onto the governing physics equation, creating a reduced model with essential physics details. We incorporate discontinuous Galerkin domain decomposition (DG-DD), enabling large-scale system construction without data at such vast scales. Applying this approach to the incompressible Stokes flow

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equation, we achieve nearly 16 times faster solutions with a relative error of $\lesssim 2\%$, even at scales 1000 times larger than the original problem.

1 Introduction

A computational framework for analyzing repeated unit cell structures under Stokes flow conditions finds application in various domains. For instance, in the realm of tissue engineering, the design of porous biomaterial scaffolds requires the solution of Stokes flow within repeated unit cell structures [1]. Another instance arises in the context of liquid composite molding processes, where solving for Stokes flow within repeated unit cell structures is a requisite step [2]. Additionally, such a framework could be applied to studying the mass transfer properties of passive and active biological particles in complex porous media [3, 4].

Extensive research has been dedicated to developing computational techniques for the accurate solution of the Stokes flow equation [5–8]. While various high-fidelity methods demonstrate effectiveness in solving small-scale systems with only a few unit cells, the computational expenses escalate significantly when attempting to scale up the system, especially with increasing number of shapes, size and configurations of unit cells. Non-dimensionalization of the problem may alleviate some of the computational burdens associated with scaling; however, achieving geometric and dynamic similarity in all scenarios is often unattainable. Consequently, there arises a need to solve the equation for system sizes that are computationally prohibitive using traditional numerical methods. A commonly employed approach is to model the unit cells using a volume-averaged approximation, although this method is known to introduce errors associated with the closure problem. [9].

In contrast to the volume-approximation approach, projection-based reduced order models (ROMs) effectively approximate the high-fidelity computational models with dominant physics modes identified from sample data [10–13]. As a result, they can minimize the impact of the approximation by neglecting only the minor details. As its variant, component-level ROMs exhibit remarkable capability in extrapolating outcomes for large-scale systems based solely on data from smaller unit cells. These component-level ROMs have been successfully employed across a spectrum of physical problems, including lattice-type structure design optimization [14, 15], microtruss structures [16], heat conduction/exchange [17–19], linear elasticity [17], and acoustic Helmholtz problems [20]. However, it is important to note that the performance of these component-level approaches hinges on their ability to accurately represent interface degrees of freedom through port interface bases. The introduction of port bases can add complexity to the implementation of these component-level methods.

To address this challenge, we propose a novel physics-constrained data-driven component-level reduced order model (ROM) that offers both speed and accuracy in predicting outcomes for large-scale systems, all without the need to introduce port interface bases. To accomplish this, we leverage a discontinuous-Galerkin domain decomposition (DG-DD) approach. The component-level ROM begins by identifying the dominant modes within a given physics system based on component-level sample data. Subsequently, the governing equations for component-level Stokes flow physics are projected onto the linear subspace defined by these identified modes, yielding a component-level reduced order model. DG-DD, on the other hand, decomposes a larger global system into smaller-scale components, where the component-level ROMs serve as foundational building blocks that are seamlessly integrated into the overarching global-scale ROM. This integrated approach allows for accurate and efficient predictions on a large scale, all while circumventing the need for port interface bases.

The rest of the paper is organized as follows. In Section 2, we provide a concise overview of the proposed component model reduction approach as it pertains to general partial differential equations (PDEs). Following that, in Section 3, we illustrate the practical application of the overarching framework discussed in Section 2 to the specific case of the Stokes flow equation.

2 General framework

We consider the global-scale domain Ω decomposed into M subdomains Ω_m, i.e. $\Omega = \bigcup_{m=1}^{M} \Omega_m$. All subdomains can be categorized into a few reference domains $\mathbb{C} \equiv \left\{\overline{\Omega}_1, \overline{\Omega}_2, \ldots\right\}$. We consider a

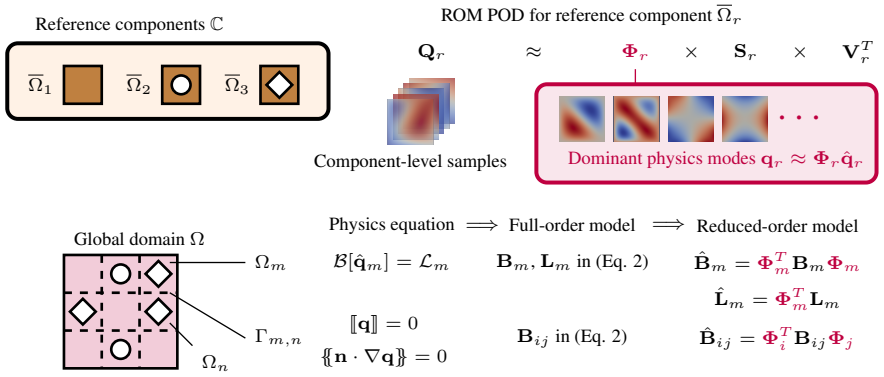


Figure 1: Illustration of component model reduction.

general linear partial differential equation for each subdomain physics state $\tilde{\mathbf{q}}_m \in H_1(\Omega_m)$,

$$\mathcal{B}[\tilde{\mathbf{q}}_m] = \mathcal{L}_m \qquad \text{in } \Omega_m, \tag{1a}$$

with the continuity and smoothness constraints on the interface $\Gamma_{m,n} \equiv \partial\Omega_m \cap \partial\Omega_n$,

$$[\![\tilde{\mathbf{q}}]\!] \equiv \tilde{\mathbf{q}}_m - \tilde{\mathbf{q}}_n = 0 \qquad \text{on } \Gamma_{m,n} \tag{1b}$$

$$\{\!\{\mathbf{n} \cdot \nabla \tilde{\mathbf{q}}\}\!\} \equiv \frac{1}{2}\left(\mathbf{n}_m \cdot \nabla \tilde{\mathbf{q}}_m + \mathbf{n}_n \cdot \nabla \tilde{\mathbf{q}}_n\right) = 0 \qquad \text{on } \Gamma_{m,n}, \tag{1c}$$

where $\mathbf{n}_m$ is the outward normal vector of Ω_m. DG-DD seeks an approximate solution $\mathbf{q} = \{\mathbf{q}_m\}$ that satisfies the discretization of (1),

$$\mathbf{B}_m \mathbf{q}_m + \sum_{\Gamma_{m,n} \neq \emptyset} \begin{pmatrix} \mathbf{B}_{mm} & \mathbf{B}_{mn} \end{pmatrix} \begin{pmatrix} \mathbf{q}_m \\ \mathbf{q}_n \end{pmatrix} = \mathbf{L}_m \qquad \forall m, \tag{2}$$

where $\mathbf{B}_m \mathbf{q}_m$ and $\mathbf{L}_m$ corresponds to the physics equation (1a), and the remaining terms to the interface condition (1b–c). This discretized physics equation provides the base for component ROM.

The component-level solution $\mathbf{q}_r$ is approximated as a combination of the dominant physics modes,

$$\mathbf{q}_r \approx \mathbf{\Phi}_r \hat{\mathbf{q}}_r, \tag{3}$$

where the reduced solution $\hat{\mathbf{q}}_r$ is essentially the coefficients of the column modes of $\mathbf{\Phi}_r$. In ROM, the proper orthogonal decomposition (POD) is used to extract $\mathbf{\Phi}_r$ from sample solutions of (1a) on the reference domain $\overline{\Omega}_r$ [21, 22]. The physics equation (2) is then projected onto the column space of $\mathbf{\Phi}_r$,

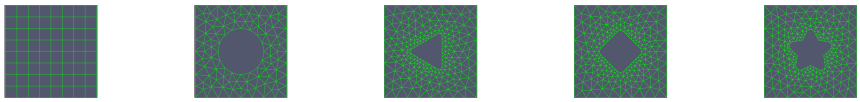
$$\hat{\mathbf{B}}_m \hat{\mathbf{q}}_m + \sum_{\Gamma_{m,n} \neq \emptyset} \begin{pmatrix} \hat{\mathbf{B}}_{mm} & \hat{\mathbf{B}}_{mn} \end{pmatrix} \begin{pmatrix} \hat{\mathbf{q}}_m \\ \hat{\mathbf{q}}_n \end{pmatrix} = \hat{\mathbf{L}}_m \qquad \forall m, \tag{4}$$

with ROM operators $\hat{\mathbf{B}}_m = \mathbf{\Phi}_m^T \mathbf{B}_m \mathbf{\Phi}_m$, $\hat{\mathbf{B}}_{ij} = \mathbf{\Phi}_i^T \mathbf{B}_{ij} \mathbf{\Phi}_j$ and $\hat{\mathbf{L}}_m = \mathbf{\Phi}_m^T \mathbf{L}_m$. These operators are the building blocks of the global ROM. Figure 1 illustrates the construction of the global ROM from the component-level samples.

It is worth emphasizing that the ROM operators $\hat{\mathbf{B}}_m$, $\hat{\mathbf{B}}_{ij}$ and $\hat{\mathbf{L}}_m$ need not be constructed from a global scale system. The POD modes $\mathbf{\Phi}_r$ can be identified from the component-level samples. The discretized operators $\mathbf{B}_m$, $\mathbf{B}_{ij}$ and $\mathbf{L}_m$ can be constructed in the reference component domains, and repeatedly used over the entire global domain. As long as the component-level samples for training $\mathbf{\Phi}_r$ are rich enough to represent general physics, the global ROM can robustly predict at larger scales in an efficient manner.

3 Demonstration

We demonstrate the component model reduction for the incompressible Stokes flow equation, where the component governing equation (1a) for $\mathbf{q}_m \equiv (\mathbf{u}_m, p_m)$ is



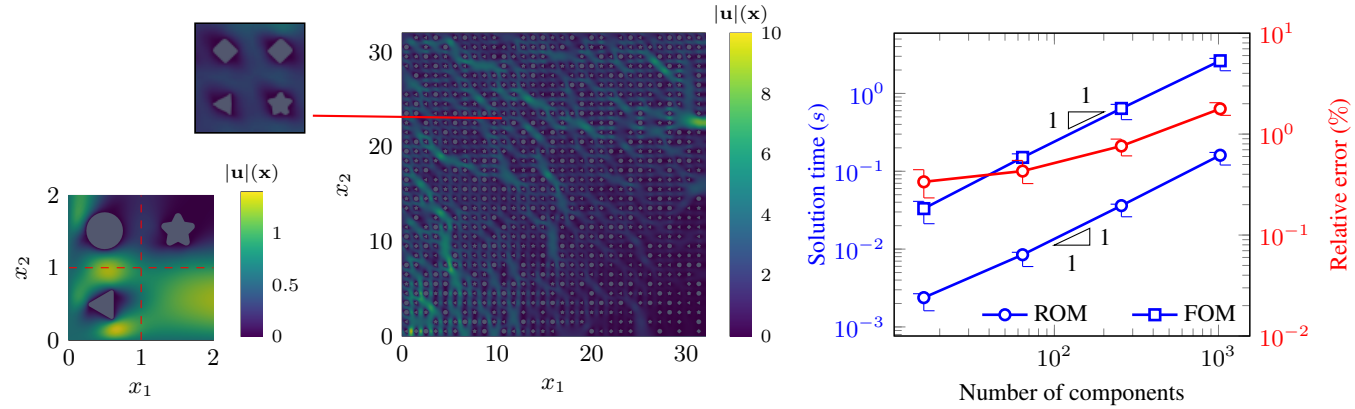
(a) $\overline{\Omega}_1$: empty (b) $\overline{\Omega}_2$: circle (c) $\overline{\Omega}_3$: triangle (d) $\overline{\Omega}_4$: square (e) $\overline{\Omega}_5$: star

Figure 2: Reference domains used as components: (a) empty, (b) circle, (c) triangle, (d) square, and (e) star.

$$-\mu\nabla^2\tilde{\mathbf{u}}_m + \nabla\tilde{p}_m = 0 \qquad \text{in } \Omega_m \tag{5a}$$

$$\nabla\cdot\tilde{\mathbf{u}}_m = 0 \qquad \text{in } \Omega_m, \tag{5b}$$

where $\mathbf{u}$ and p denotes the velocity and pressure field, respectively and $\mu = 1.1$ is the dynamic viscosity. (5) describes the conservation of momentum with incompressibility condition.



(a) Component level sample (b) Global level prediction (c) Performance

Figure 3: Component model reduction for the Stokes flow equation: (a) a sample data with a random inflow condition; (b) a prediction made by the global ROM; and (c) the computation time and relative error of the ROM solution compared to the full-order model (FOM). The computation time and the relative error are measured over 100 different inflow conditions.

Five different reference domains $\mathbb{C} = \{\overline{\Omega}_1, \ldots, \overline{\Omega}_5\}$ are considered as components for building up the global-scale system. All reference domains lie within a unit square $\overline{\Omega}_r \subset [0,1]^2$, with or without an obstacle within them, as shown in Figure 2. The type and number of elements of each component is summarized in Table 1. The full order model (FOM) discretization (2) is implemented for (5)

$\overline{\Omega}_r$ (name)	$\overline{\Omega}_1$ (empty)	$\overline{\Omega}_2$ (circle)	$\overline{\Omega}_3$ (triangle)	$\overline{\Omega}_4$ (square)	$\overline{\Omega}_5$ (star)
Number of elements	64	168	393	372	415
Number of samples	1115	1076	1098	1114	1197

Table 1: Specification of component reference domains.

in the `MFEM` framework [23]. To develop the ROM, 1400 sample snapshots for basis training are generated on 2-by-2-component domains. For each sample, the domain is constructed with four randomly chosen subdomains from $\mathbb{C}$. On each sample domain, a random inflow velocity is set with a sinusoidal perturbation for the Dirichlet boundary condition,

$$\mathbf{u}_{di} = (g_1 + \Delta g_1 \sin 2\pi(\mathbf{k}_1\cdot\mathbf{x} + \theta_1), g_2 + \Delta g_2 \sin 2\pi(\mathbf{k}_2\cdot\mathbf{x} + \theta_2)), \tag{6}$$

on the Dirichlet boundary $\partial\Omega_{di}$, which is the upwind sides of Ω. The parameters in (6) are chosen from uniform random distributions for each sample. At the surface of the object inside the domain, a no-slip wall boundary condition is set, and the rest of the boundary is set as a no-stress outflow

condition. Figure 3 (a) shows an example sample domain and its velocity magnitude. From these samples, 36 POD modes are identified and the global ROM is constructed for larger-scale domains, up to $M = 1024$-component system. Figure 3 (c) shows the computation time and the relative error of the ROM at different M. At each size, the ROM prediction is made for 100 cases of random inflow conditions and compared with the FOM. The resulting global ROM reduced the computation time by a factor of 16, up to 1024-component systems. The accuracy of the prediction, however, is not compromised. The relative error of the ROM is maintained at $\lesssim 2\%$ over all scales. It is worth emphasizing that the ROM exhibits a consistent performance over all cases of inflow conditions, all of which are highly extrapolative. Figure 3 (b) shows a global ROM prediction for a random 32-by-32-component system, where the velocity magnitude is 10 times larger than those of the sample data. Nonetheless, the accuracy of the ROM is robustly maintained.

4 Conclusion

In this work we address a common practical challenge in scaling up, where the data for the model reduction is provided only at small component-level scales, and accurate prediction is required at a much larger scale. We developed a component ROM where the ROM is combined with DG-DD. The proposed method provides building blocks for robust and efficient prediction at an extrapolated scale.

The proposed method is demonstrated on the Stokes flow equation. The resulting ROM accelerates the solving time by a factor of 16, for global domains up to 1000 times larger than the component domains. The resulting ROM was capable of robust prediction without compromising the accuracy, as demonstrated by the small relative error ($\lesssim 2\%$) over all scales. In this study, the reference domains are chosen to lie within a simple unit square for the demonstration. However, the proposed method is not limited to certain geometries: any shape of reference domain can be chosen as long as its interface is conforming to other reference domains.

It is well known that the linear subspace ROM cannot be naively applied to the nonlinear problems. In case of polynomially nonlinear PDEs such as incompressible Navier–Stokes flow, the tensorial approach can be applied [24]. In other cases, hyper-reduction approaches are also available [25–29]. In all cases, similar ROM variants can be formulated with the DG-DD, as all the model reduction techniques similarly exploits the physics equation.

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