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On a sparse pressure-flow rate condensation of rigid circulation models

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ABSTRACT

Cardiovascular simulation has shown potential value in clinical decision-making, providing a framework to assess changes in hemodynamics produced by physiological and surgical alterations. State-of-the-art predictions are provided by deterministic multiscale numerical approaches coupling 3D finite element Navier Stokes simulations to lumped parameter circulation models governed by ODEs. Development of next-generation stochastic multiscale models whose parameters can be learned from available clinical data under uncertainty constitutes a research challenge made more difficult by the high computational cost typically associated with the solution of these models. We present a methodology for constructing reduced representations that condense the behavior of 3D anatomical models using outlet pressure-flow polynomial surrogates, based on multiscale model solutions spanning several heart cycles. Relevance vector machine regression is compared with maximum likelihood estimation, showing that sparse pressure/flow rate approximations offer superior performance in producing working surrogate models to be included in lumped circulation networks. Sensitivities of outlets flow rates are also quantified through a Sobol' decomposition of their total variance encoded in the orthogonal polynomial expansion. Finally, we show that augmented lumped parameter models including the proposed surrogates accurately reproduce the response of multiscale models they were derived from. In particular, results are presented for models of the coronary circulation with closed loop boundary conditions and the abdominal aorta with open loop boundary conditions.

1. Introduction

Three-dimensional simulations of vascular hemodynamics are widely used, with increasing clinical implication, in applications ranging from pediatric cardiology to coronary artery and aneurysm hemodynamics. Before these models can be used to complement clinical decision making, vascular geometry, material properties and boundary conditions need to be estimated from clinical data. Unfortunately, the significant computational cost of simulations severely limits the use of parameter estimation, uncertainty quantification and optimization procedures, all requiring repeated model evaluations needed to produce reasonable patient-specific estimates of model parameters. We argue that such characterization of model parameters should also be determined stochastically, producing associated confidence metrics on simulation results. This typically leads to a further increase in the number of simulations needed, for example, in Bayesian estimation approaches.

Multiscale cardiovascular models (see, e.g., Formaggia et al., 2001; Moghadam et al., 2013), for example, couple three-dimensional discrete finite element simulations with 1D or lumped parameter descriptions of the patient circulation. Lumped parameter models, obtained by linearizing the Navier–Stokes equations around rest conditions (Milišić and Quarteroni, 2004), are formulated through systems of ODEs analogous to those describing the evolution of current and voltage in an electrical circuit and belong to two main families, i.e., open or closed loop boundary conditions. Open loop boundary conditions (see, e.g., Vignon-Clementel et al., 2006) are circuit models, such as RCR, that are applied at each outlet face and end at ground, while closed loop boundary conditions (see, e.g., Corsini et al., 2014) connect back to the model inlet to mimic the entire circulation. We will refer to the latter models as *circulation* or *LPN* models in what follows. Similar systems can also be assembled by coupling 3D CFD models with 1D peripheral counterparts. While techniques for parameter estimation and data assimilation in lumped circulation networks have been proposed in the literature (see, e.g., Spilker and Taylor, 2010; Revie et al., 2013; Sughimoto et al., 2013; Yu

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et al., 2001; Xiao et al., 2002; Deswysen, 1977; Clark et al., 1980; Deswysen et al., 1980; McInnis et al., 1985; Shimooka et al., 1991; Avanzolini et al., 1992; Ruchti et al., 1993; Yu et al., 1998), the computational cost of solving the coupled 0D/3D problem has prevented extension of these techniques to multiscale models.

A viable approach to overcome this difficulty is to construct a *reduced order model* that can replace a full finite element solution at a fraction of the computational cost. A significant number of contributions on this topic can be found in the literature and the list that follows is by no means comprehensive.

A review of reduced order modeling approaches is presented in Benner et al. (2013) addressing and comparing model reduction techniques for non-parameterized and parameterized systems developed in the proper orthogonal decomposition (POD) and the control theory communities, respectively. It discusses computing the trial and test spanning sets for Petrov–Galerkin projection basis using three approaches, rational interpolation, balanced truncation and POD. Strategies for sampling in parameter space to minimize errors between the original high-fidelity model and its reduced order representation are also critically reviewed.

An extensive treatment of reduced basis approximations for affinely parameterized elliptic coercive partial differential equations is presented in Rozza et al. (2008), where the authors discuss an online–offline projection of a full finite element solution onto the space generated by solution snapshots identified through greedy sampling strategies. A review of recent developments in this direction is also presented in Chen et al. (2015).

In the context of interpolatory approximation of the response functions for general SISO (single-input, single-output) and MIMO (multiple-input, multiple-output) systems, an extensive review can be found in Antoulas et al. (2010), also addressing situations where the Loewner data-driven framework is used for high-fidelity systems characterized through a reduced number of inputs and outputs. A recent contribution, in this context, discusses the development of rational macro-models for one-dimensional blood flow in arteries (Ferranti et al., 2015).

Balanced truncation approaches are reviewed in Gugercin and Antoulas (2004), while a vast literature is available on POD methods, starting from the first applications to turbulent flow in the late 60s to more recent developments (see, e.g., Berkooz et al., 1993; Rowley, 2005).

Finally, additional recent work on reduced order modeling with cardiovascular applications can be found in McLeod et al. (2010), Guibert et al. (2014), Colciago (2014), and Ballarin (2015).

Our approach separates the finite element model and its boundary circulation network in two systems with coupling occurring at the interface, where pressure/flow rate information is (implicitly or explicitly) exchanged at every solution time step. In particular, the LPN model receives outlet flow rates from the finite element model and provides pressures back to the same outlets for the next time step. Conversely, the 3D model receives outlet pressures from the LPN and provides updated local distributions of pressure and velocities, resulting in new outlet flow rates. This way of representing a multiscale model, i.e., consisting of two subsystems continuously exchanging pressure/flow rate information, inspires model reduction approaches that preserve the exchange of information at the interface. We therefore propose a methodology for building outlet pressure-flow rate approximants of discrete models. We demonstrate that use of sparse regressors is paramount to building condensed representations that can be successfully integrated into ODE solvers for boundary circulation models.

The problem of constructing a pressure/flow rate surrogate of a discrete anatomical model is presented in Section 2, formulated as an orthogonal multivariate polynomial regression problem. We also discuss the main assumptions behind this approach, mainly related to treatment of inertia and compliance phenomena. Section 3 presents two methodologies for estimating the expansion coefficients, namely maximum likelihood estimation through Ordinary Least Squares (OLS see, e.g., Banks et al., 2014) and Relevance Vector Machine regression (RVM) (Tipping, 2001; Tipping et al., 2003). Pressure-flow surrogates are constructed in Section 4, while Section 5 shows how outlet flow rate sensitivities and amplification of pressure perturbations though the approximant are affected by constraining the sparsity of the resultant representation. Finally, conclusions are presented in Section 6.

2. Problem statement

Consider a region $\Omega \subset \mathbb{R}^3$ occupied by a three-dimensional representation of the vasculature. The boundary of Ω is denoted by $\partial\Omega$ and partitioned into the following disjoint sets: *walls* $\mathbf{\Gamma}^w = \{\Gamma_j^w, j = 1, \ldots, n_w\}$, *inlets* $\mathbf{\Gamma}^i = \{\Gamma_j^i, j = 1, \ldots, n_i\}$ and *outlets* $\mathbf{\Gamma}^o = \{\Gamma_i^o, i = 1, \ldots, n_o\}$. In what follows, the set $\mathbf{\Gamma} = \{\Gamma_j, j = 1, \ldots, n\}$ will be used to generically refer both to model inlets or outlets or, in other words, $\mathbf{\Gamma} = \mathbf{\Gamma}^i \cup \mathbf{\Gamma}^o$ and $n = n_i + n_o$. Average pressures and flow rates at the generic Γ_i are characterized using the random vectors $\mathbf{p} = (p_1, \ldots, p_n) \in \mathbf{\Lambda}_p \subset \mathbb{R}^n$ and $\mathbf{q} = (q_1, \ldots, q_n) \in \mathbf{\Lambda}_q \subset \mathbb{R}^n$ with joint distribution $\rho(\mathbf{p})$ and $\rho(\mathbf{q})$, respectively, defined over the probability triplet $(\Xi, \mathcal{F}, \mathcal{P})$. Here, Ξ is the sample space, $\mathcal{F}$ is a σ-algebra of possible events, and $\mathcal{P}$ denotes a probability measure on $\mathcal{F}$. The generic average outlet pressure p_i and flow rate q_i are also defined as follows:

$$p_i = \frac{1}{|\Gamma_i|}\int_{\Gamma_i} p \, d\Gamma_i, \quad q_i = \int_{\Gamma_i} (\mathbf{v} \cdot \mathbf{n}_i) \, d\Gamma_i, \tag{1}$$

where p and $\mathbf{v}$ are the 3D model pressure and velocity field, respectively, while $\mathbf{n}_i$ is the normal to the interface Γ_i, assumed planar. We assume that the discrete 3D model can be replaced by a relationship between pressures and flow rates of the form:

$$q_i(t) = f(\mathbf{p}, t, \boldsymbol{\gamma}) = \sum_{j=1}^{n_b} \alpha_{j,i}(t, \boldsymbol{\gamma})\phi_j(\mathbf{p}, t, \boldsymbol{\gamma}), \quad i = 1, \ldots, n. \tag{2}$$

where t represents time, $\boldsymbol{\alpha}_i = (\alpha_{1,i}, \ldots, \alpha_{n_b,i}) \in \mathbb{R}^{n_b}$ is a vector of expansion coefficients characterizing the flow rate at the generic Γ_i, ϕ_j is a set of basis functions (yet to be chosen, see next paragraph) with cardinality n_b, assuming values over $\mathbf{p}$, t and $\boldsymbol{\gamma}$, a vector of additional variables. A possible example of additional variables in $\boldsymbol{\gamma}$ is the total model volume (initial model volume plus net flow rate through the model integrated over time) in deformable wall simulations. At this point, we assume independence from t and $\boldsymbol{\gamma}$ in (2). The first assumption, time independency, holds in situations characterized by limited inertia effects. We refer the reader to Section 2.1 for a discussion on the contribution of inertance to the pressure drop for two extreme vessel geometries and physiological flow conditions. The second assumption is instead related to the choice of rigid wall models. Although the approach presented in the next sections can be extended to deformable wall models by properly introducing additional variables, we leave the demonstration of this to future studies. The expansion in (2) can therefore be simplified to:

$$q_i = \sum_{j=1}^{n_b} \alpha_{j,i} \, \phi_j(\mathbf{p}), \quad i = 1, \ldots, n. \tag{3}$$

Multivariate Legendre polynomials combined with a linear transformation to $[-1, 1]$ are used, in this work, as the basis functions $\phi_j, j = 1, \ldots, p$. These polynomials are orthogonal with respect to a uniform weight function $w(x_i) = 0.5, x_i \in [-1, 1] \subset \mathbb{R}$, and satisfy