Journal of Computational Science 4 (2013) 101–110

Contents lists available at SciVerse ScienceDirect

Journal of Computational Science

journal homepage: www.elsevier.com/locate/jocs

A rapid interpolation method of finding vascular CFD solutions with spectral collocation methods

Jae-Hun Jung [a,*], Joseph Lee [b], Kenneth R. Hoffmann [b], Todd Dorazio [b], E. Bruce Pitman [a]

[a] Department of Mathematics, State University of New York at Buffalo, Buffalo, NY 14260-2900, USA
[b] Department of Neurosurgery, State University of New York at Buffalo, Buffalo, NY 14260-2900, USA

ARTICLE INFO

Article history:
Received 6 February 2012
Received in revised form 18 May 2012
Accepted 4 June 2012
Available online 20 June 2012

Keywords:
Rapid computational fluid dynamics
Homeomorphic mapping
Polynomial interpolation
Vascular flows
Spectral collocation methods

ABSTRACT

We propose a rapid interpolation method of computational fluid dynamics (CFD) solution based on the collocation method for vascular flows through the polynomial interpolation and present a *proof-of-concept* computation of our preliminary results. A rapid CFD can play a crucial role for some applications such as the hemodynamics assessment for human vasculature in the emergent situation. The CFD approach for the real-time assessment at the clinical level is, however, not a practical tool due to the computational complexity and the long time integration needed for the individual CFDs. We propose an efficient, accurate, yet fast interpolation method of finding CFD solutions that can be utilized for the real-time hemodynamic analysis for clinicians. The main idea of the method is to use the vascular library where vascular solutions with different parameter values are pre-computed and stored. The desired unknown CFD solution is obtained via the interpolation using the similar solutions from the library. We use the spectral collocation method for the individual CFD solutions. The collocation method makes it easier to map the solution from the physical domain to the reference domain for the interpolation using the homeomorphic transformation. The interpolation is then directly constructed using the solution fields at the collocation points. Our preliminary results for vascular flows of 3D stenosis show that the proposed method is fast and accurate.

1. Introduction

The main purpose of this paper is to propose a simple interpolation method of finding computational fluid dynamics (CFD) solution on the collocation points via the solution library concept and provide the *proof-of-concept* computation of our preliminary results. The proposed method is to obtain a fast CFD solution without running the actual CFD simulations of the individual solutions. The motivation is from the persistent demand that the fast and accurate hemodynamic evaluation of human vasculature is crucial for the reliable vascular assessment in the emergent situation to save human lives. The real-time CFD computation is not an option for clinicians in the emergent situation due to its computational complexity. To avoid the actual CFD computation and obtain the accurate unknown CFD solution extremely fast, we propose to use the CFD library where the individual CFD solutions with different parameter values are pre-computed and stored and use those pre-computed CFD solutions as the interpolation basis for the unknown CFD solution.

Similar ideas were already proposed such as the reduced basis method (RBM) [14,15,18,19]. The basic framework of the RBM is the proper mapping from the physical frame to the reference frame where the actual computational approximation is carried out. In literature, the RBM method was realized based on the finite element method (FEM) [13] or the discontinuous Galerkin (DG) method [3] for which the local or global basis functions are mapped according to the geometric deformation. The parameters that determine the mapping are plugged into the given partial differential equations (PDEs) and the new equations containing the parameters are derived. If the sample solutions are pre-computed, they are used for the unknown solution as the approximation basis according to the derived equations. Some of recent works of RBM can be also found in the special issue of ICOSAHOM 2009 [3,8,13].

We propose a more direct approach using the collocation approach. That is, the unknown solution is approximated directly via the standard interpolation scheme using the physical values defined on the collocation points. If the given parameter value is associated with the geometry, the pre-computed physical solutions on the collocation points are mapped into the reference frame via the homeomorphic mapping and the unknown solution is directly approximated via the interpolation. The homeomorphic mapping

* Corresponding author. Tel.: +1 716 645 8814.
E-mail addresses: jaehun@buffalo.edu (J.-H. Jung), jwlee6@buffalo.edu (J. Lee), kh9@buffalo.edu (K.R. Hoffmann), tdorazio@buffalo.edu (T. Dorazio), pitman@buffalo.edu (E.B. Pitman).

1877-7503/$ – see front matter
http://dx.doi.org/10.1016/j.jocs.2012.06.001

is applied for the problem that has the topological equivalence for its individual solutions. If the parameter is not associated with the geometry, the interpolation is even more straightforward without any geometric mapping. We can adopt the pre-existing interpolation schemes such as the standard polynomial interpolations and radial basis function (RBF) interpolations [2] to utilize the proposed method.

For the proposed method, we assume the following:

(1) There exists an interval of non-zero measure in the *parameter space* where the parameter values of the associated unknown solution exist.
(2) In such an interval, the function varies smoothly so that the solution fields also vary smoothly without a discontinuity. This yields a well-defined interpolation.
(3) We can refine the interval if necessary.

With these assumptions, once we find such intervals where the solution is smooth and we know a priori that the unknown solution is defined by the parameters that exist in the found interval, the unknown solution can be found via a simple interpolation method such as the polynomial interpolation.

There are couple of issues that should be carefully investigated further, which we do not attempt to resolve in this paper but leave as our future research subjects:

(1) Adaptive re-sampling technique: if the smooth interval is found, such an interval can be refined using the re-sampling method and the corresponding pre-computed CFD solutions are identified accordingly. The re-sampling not only increases the degree of accuracy but also avoids the ill-conditioning of the interpolation matrix and the possible Runge effect.
(2) Metric measurement: for vascular flows, the metric quantities are more important than the physical variables that appear in the governing equations. These metrics include the vorticity, the degree of recirculation, the on-set of turbulence, etc. The metric quantities enable the smooth intervals to be found efficiently. For example, if there exists a bifurcating point in the parameter space, the interpolation across the bifurcation point will provide a poor convergence to the desired solution due to the possible jump discontinuity in the pre-computed solution basis. For this case, the corresponding metric quantity helps separate the region so that the new interval for the interpolation does not contain the bifurcation point.
(3) Fast search algorithm: when multiple parameters are involved, a fast search algorithm of the similar CFD solutions to the given parameter values of the unknown CFD solution is needed.
(4) The interpolation scheme for the time-dependent problems: for our preliminary research we focus on the steady-state solutions, but the proposed method is still applicable. For the time-dependent pulsatile flows the proposed method can be applied to few sample solutions within the pulsatile period.
(5) Extremely high value of percent stenosis: there may be a mathematical bifurcation in the linearity of the solutions when percent stenosis becomes extremely high. If recirculations become dominant and bifurcation occurs, the re-sampling method should be applied to have the interpolation well defined.

Leaving all these issues in our future work, we consider a simple model of the 3D stenotic CFD based on the collocation method and interpolate the unknown solution directly on the collocation space. The preliminary results are provided. To explain the simple interpolation procedure, we first use the simple 1D and 2D examples.

The paper is composed of the following sections. In Section 2, we explain the incompressible Navier–Stokes equations as the governing equations for vascular flows and the multi-domain spectral collocation method is explained to approximate the governing equations. In Section 3 we explain the solution library and the homeomorphic transformation to map the obtained CFD solutions into the reference domain where the interpolation is made for the unknown CFD solution. Section 4 explains the interpolation methods to find the unknown CFD solution using the similar CFD solutions from the solution library. Section 5 provides the preliminary numerical results. Section 6 provides a brief conclusion.

2. Governing equations and numerical methods

2.1. Incompressible Navier–Stokes equations

For the vascular flow equations, we use the Eulerian representation of flows with density $\rho = \rho(\mathbf{x}, t)$, pressure $P = P(\mathbf{x}, t)$, and velocity vector $\mathbf{u} = (u, v, w)^T$, for $\mathbf{x} = (x, y, z)^T \in \Omega$, $t \in \mathbb{R}^+$, where Ω is the closed domain of vascular fluid, $\Omega \subset \mathbb{R}^3$, and u, v, and w are the component of $\mathbf{u}$ in x, y, and z directions, respectively [20]. We assume that the blood flow is Newtonian. Such an assumption does not precisely describe the exact behavior of vascular flows, but the Newtonian assumption suffices for the purpose of our work. We assume the smoothness of flows in the parameter space and do not consider extreme geometries. Then the governing equations are given by the Navier–Stokes equations with the mass conservation laws

$$\rho(\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u}) - \mu\Delta\mathbf{u} - (3\lambda + \mu)\nabla(\nabla\cdot\mathbf{u}) + \nabla P = f, \tag{1}$$

$$\rho_t + \nabla\cdot(\rho\mathbf{u}) = 0, \tag{2}$$

where $\mu \in \mathbb{R}^+$ is the kinematic viscosity, $\lambda \in \mathbb{R}$ is a constant and f denotes the external force of blood flows. Further, we assume that the blood flow is homogeneous both in $\mathbf{x}$ and t and incompressible. That is, $\rho = \rho_o > 0$ is a non-zero constant for all $\mathbf{x}$ and t. Also, we assume that there is no external force, such as $f = \mathbf{0}$. Then we have

$$\rho(\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u}) - \mu\Delta\mathbf{u} + \nabla P = \mathbf{0}, \tag{3}$$

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

Here for numerical convenience, we use the nondimensionalization of the above equation. For the nondimensionalization, we use the physical and geometrical parameter values of the normal blood. These are the length scale $x_o = 0.26$, the unit velocity $u_o = 30$, the time scale $t_o = 6.7 \times 10^{-3}$, the unit pressure $P_o = 900$, the unit density $\rho_o = 1$, and the unit kinetic viscosity $\mu = 0.0377$ (all in *cgs* units). Then the nondimensionalized incompressible Navier–Stokes equations are given by

$$\begin{aligned} &\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} - \nu\Delta\mathbf{u} + \nabla p = 0, \\ &\nabla\cdot\mathbf{u} = 0, \end{aligned} \tag{5}$$

where we can consider each variable as the scaled variable by the reference values given above. For example, $\rho = \rho'/\rho_o$ where $'$ denotes the variable in Eq. (3) and $p = P'/\rho_o$. The constant ν can be considered as the Reynolds number of the flow, that is,

$$1/\nu = \mathrm{Re} = \frac{\rho_o x_o u_o}{\mu}. \tag{6}$$

Projection method: There are different ways of solving Eq. (5). One of them is the *projection* method [5,20], for which the intermediate velocity field is first solved using the convection and diffusion parts of the equation. Then by the incompressibility condition $\nabla\cdot\mathbf{u} = 0$, the pressure is obtained using the Poisson equation. The intermediate velocity fields are again updated using the obtained pressure.