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A Scalable Domain Decomposition Method for Ultra-Parallel Arterial Flow Simulations[†]

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Abstract. Ultra-parallel flow simulations on hundreds of thousands of processors require new multi-level domain decomposition methods. Here we present such a new two-level method that has features both of discontinuous and continuous Galerkin formulations. Specifically, at the coarse level the domain is subdivided into several big patches and within each patch a spectral element discretization (fine level) is employed. New interface conditions for the Navier-Stokes equations are developed to connect the patches, relaxing the C^0 continuity and minimizing data transfer at the patch interface. We perform several 3D flow simulations of a benchmark problem and of arterial flows to evaluate the performance of the new method and investigate its accuracy.

AMS subject classifications: 52B10, 65D18, 68U05, 68U07 **Key words**: Bioflows, spectral elements, discontinuous Galerkin, parallel computing.

1 Introduction

Current and projected advances in computer architectures involving hundreds of thousands of processors cannot be exploited for large-scale simulations of the human arterial tree [1,2] (or of many other physical and biological problems) based on existing domain decomposition algorithms and corresponding parallel paradigms. Not only we have to address the tremendous complexity associated with data transfer amongst thousands of processors, but more fundamentally the solution of linear systems with billions degrees of freedom (DOFs) and corresponding condition number exceeding one million is a rather formidable task.

In this paper we develop a significant extension of the spectral/*hp* element method (SEM) for large-scale simulation of arterial blood flow dynamics. In particular, we adopt

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⁺Dedicated to Professor Xiantu He on the occasion of his 70th birthday.

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two levels of discretization by introducing coarse-level patches to decompose the computational domain. SEM, similarly to finite element method, is based on discretization of the computational domain into non-overlapping elements. Within each element the solution is approximated with a high-order (spectral) polynomial expansion. The total number of DOFs depends on the number of elements and the order of polynomial expansion within each element. The two common approaches for solution of partial differential equations with SEM are [3]: (a) Discontinuous Galerkin method (DG), where discontinuity of the numerical solution at the interfaces of elements is allowed; and (b) Continuous Galerkin method, where the boundary degrees of freedom defined at the interfaces of elements are shared, hence enforces C^0 continuity of the numerical solution. In the C^0 approximation global linear operators are constructed from the local ones by static condensation and due to sharing of the boundary degrees of freedom the rank of the global operator is lower than the total number of local DOFs.

In 3D large-scale simulations, the number of spectral elements can be well over a million, and due to the high-order polynomial expansion the number of DOFs may be over several billions. For example, the aorta domain in Fig. 1 has 325,795 tetrahedral elements and includes only 17 arteries while a domain to discretize 65 major cranial arteries [4] has 459,250 tetrahedral elements. To resolve the complex patterns of unsteady blood flow such as secondary flows, turbulence and recirculation, high-order spatial resolution is required. Hence, in the aorta domain employing sixth-order polynomial expansions leads to 187,657,920 number of unknowns per variable[§] while in the cranial domain it leads to 264,528,000 number of unknowns. In bigger domains with 10 millions elements and sixth-order polynomial approximation the number of unknowns for each variable would be 5.76 billions or more than 20 billions DOFs for all four variables (3D velocity vector plus pressure).

This large number of unknowns leads to construction of a global linear operator matrix with very high rank and consequently with very large condition number. Decoupling of the interior degrees of freedom by applying Schur decomposition leads to reduction in the size of the linear operator that must be inverted, however, the rank of the Schur complement is still very large. In the current study we use the parallel solver NEKTAR [5], which employs a Preconditioned Conjugate Gradient (PCG) algorithm to solve the four linear systems for the velocity and pressure. Among the different preconditioners we have tested for parallel computations, the so-called Low Energy Basis Preconditioner (LEBP) [6–8] is the most effective. In Fig. 2 we plot the performance of NEKTAR (using LEBP) on the CRAY XT3 for a simulation involving 120,813 elements. The scaling is favorable for high-order polynomial approximation. In the parallel LEBP the coarse linear vertex preconditioner is implemented in two steps: In the first step, the global operator constructed from the linear (vertex) modes, which are shared by different partitions, is constructed and inverted in parallel. In the second step, the local operator constructed from linear modes within each partition is inverted. The size of the global operator is

[§]Here we define the number of unknowns as the number of quadrature points required for exact integration of the linear terms in the Navier-Stokes equation.