Parallel Implementation of a Hybrid Particle-Continuum Finite Element Framework for Blood Clot Biomechanics

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***Abstract*—Pathological blood clotting is the primary cause of major cardiovascular diseases. Here we present a distributed-memory parallelized implementation of a hybrid particle-continuum fictitious domain finite element framework which is used to study flow and transport around a pathologically formed blood clot (thrombus). Understanding how clot shape and microstructure affect transport of proteins and drug is essential for treatment of such disease. Our particle-continuum approach represents a clot as an aggregate of discrete particles. The particle aggregate is projected onto a background fluid grid as fictitious domain data, and communicated in accordance with mesh partitions across the distributed memory processes. We have illustrated details of the parallel implementation using a parametric study of 2D transient hemodynamics, and a 3D mesh-refinement study.**

***Index Terms*—fictitious domain, finite element, blood clots, distributed memory, mesh refinement.**

I. Introduction

Pathological blood clotting, or thrombosis, is the primary cause of major cardiovascular diseases like stroke and heart attack. Comprehensive assessment of flow and flow-mediated transport in the clot neighborhood is critical for understanding disease progression and planning effective therapy. Realistic human blood clots have arbitrary shape and heterogeneous microstructure. Robust modeling of clot-hemodynamics interactions while accounting for the complex morphology and heterogeneity of a realistic human clot remains a challenge.

To address this challenge, we have devised a hybrid particle-continuum based finite element approach where a realistic clot is represented by an aggregate of discrete particles [1]. The particle aggregate is implicitly imposed over the fluid domain and coupled via a fictitious force accounting for clot-fluid interaction. Our approach geometrically decouples clot domain from the fluid mesh, and the particle description allows for a robust variation of clot shape and microstructure. We have implemented this approach within a finite element library FEniCS [2]. The resulting framework can effectively enable rapid parametric investigations of transient hemodynamics in the vicinity of realistic blood clots.

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However, parallel performance and scalability are important when studies on clots in realistic physiological conditions are performed. Here, we specifically investigate aspects of a distributed-memory parallel implementation of our fictitious domain approach, and illustrate key performance aspects.

II. Hybrid particle-continuum based finite element framework

Blood clot size and geometry data obtained from medical or microscopy imaging was fed into a tessellation based algorithm which formed the basis for a discrete particle reconstruction of the clot. This discrete particle aggregate was embedded onto a background unstructured mesh of the flow domain. Blood flow around this aggregate was modeled using a Petrov-Galerkin stabilized finite element method [3]. In this work, blood was assumed to be a Newtonian fluid. The resulting variational formulation of the incompressible Navier-Stokes equations is given as follows:

$$\begin{aligned}&\rho\left(\underline{\mathbf{w}}, \frac{\partial \underline{\mathbf{u}}}{\partial t}\right)_{\Omega} + \rho(\underline{\mathbf{w}}, \underline{\mathbf{u}} \cdot \nabla \underline{\mathbf{u}})_{\Omega} + (\underline{\underline{\mathbf{T}}}, \nabla \underline{\mathbf{w}})_{\Omega} \\ &- (q, \nabla \cdot \underline{\mathbf{u}})_{\Omega} + \left(\tau(\underline{\mathbf{u}}^h \cdot \nabla \underline{\mathbf{w}}^h), R^h\right)_{\Omega^h} + (\tau \nabla q^h, R^h)_{\Omega^h} \\ &+ (\underline{\mathbf{w}}, \kappa(\underline{\mathbf{u}} - \underline{\mathbf{v}}_0))_{\Omega} = 0\end{aligned} \tag{1}$$

where $(a, b)_{\Omega} \equiv \int a \cdot b d\Omega$; $\underline{\mathbf{u}}$ and p are the flow velocity and pressure respectively; $\underline{\mathbf{w}}$ and q are the velocity and pressure test functions respectively; $\underline{\underline{\mathbf{T}}}$ is the Newtonian incompressible fluid stress tensor; R^h is the residual of the momentum equation; and τ is the Petrov-Galerkin stabilization parameter as specified in [1].

The final term in (1) represents the coupled interaction between the clot and the fluid domain which constrains the local fluid velocity ($\underline{\mathbf{u}}$) to the local thrombus velocity ($\underline{\mathbf{v}}_0$). The penalty parameter κ is a pointwise discontinuous parameter which takes on a non-zero value based on the local element size h if the point is within the clot domain (Ω_T):

$$\kappa = \begin{cases} c_1 \max\left(\rho \frac{\|\underline{\mathbf{u}} - \underline{\mathbf{v}}_0\|}{h}, \frac{\mu}{h^2}\right) & \underline{\mathbf{x}} \in \Omega_T \\ 0 & \underline{\mathbf{x}} \notin \Omega_T \end{cases} \tag{2}$$

For a distributed-memory parallel implementation, the particle aggregate data for the clot was broadcasted over distributed memory processes, and the fictitious coupling term (2) was evaluated in accordance with the local mesh partition. Evaluating the coupling term essentially involves a series of in/out checks for the particles in the clot. If the thrombus is stationary, these checks can be computed locally within each mesh partition, thus requiring no additional inter-processes communications and improving performance.

III. Results

A. Parallel implementation shows good scaling

Preliminary benchmark simulations of 3D pulsatile flow around a stationary arterial blood clot was performed on a 4.8 million elements unstructured mesh, and a clot discretized using 25,000 particles. Simulations were run on the RMACC Summit cluster at CU Boulder [4]. This is a heterogeneous supercomputing cluster with IBM GPFS scratch filesystem, and an Omni-Path HFI interconnect. Our model was run on Intel Xeon E5-2680 v3 processors and showed very good strong scaling behavior up to 120 cores.

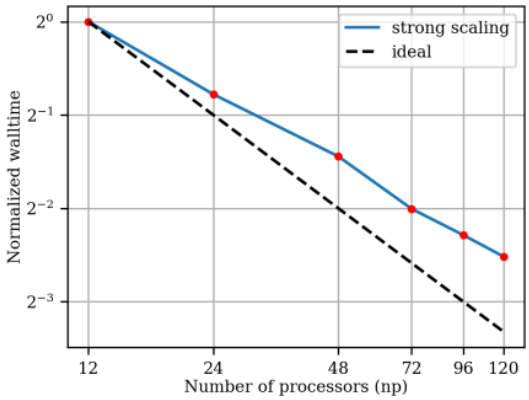

Fig. 1. Strong scaling performance of the hybrid particle-continuum finite element approach for 3D arterial clot simulations.

B. Framework enables rapid comprehensive parametric investigations

We used the parallelized implementation to conduct a systematic study of flow and transport phenomena around arterial clots; considering 2 clot shapes, 6 clot microstructures, and 4 arterial wall disease states. The resulting 48 different flow simulations were rapidly configured and computed which would not be feasible if individual cases used serial computation. The ability to conduct such parametric simulations helped quantify the significance of clot shape, microstructure, and wall disease state in key phenomena like advective transport of coagulation proteins and permeation of anticoagulant drug. Fig. 2 shows a sample set of flow data for 8 of these configurations. Our simulations indicate that macroscale flow patterns outside the clot are minimally influenced by microstructure.

C. Mesh vs particle size ratio: a key computational performance determinant

Unlike macroscale flow, flow inside the clot is strongly microstructure dependent. While the fluid mesh does not need

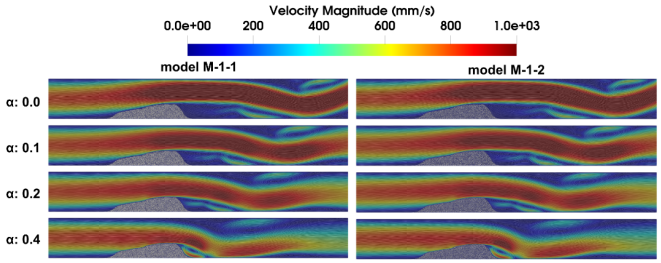

Fig. 2. Velocity field at peak systole for two different clot microstructures, and varying wall disease states (α). Flow patterns show minimal variations between different microstructures.

to conform to clot domain, some degree of mesh refinement is required in the clot domain to properly capture the interstitial flow. Specifically, too much refinement in clot interior will affect cost and performance, while too little will insufficiently resolve the microscale flow. In our implementation, this can be tuned by comparing the probability density function (pdf) of mesh element circumradii in the clot domain with the pdf of the discrete particle radii. Using a 3 dimensional simulation for a clot imposed in a simplified carotid artery model, we demonstrate how this influences solution quality. Fig. 3 left panel shows the pdf comparison for 4 successively refined meshes, with the corresponding interstitial flow solution in the inset. On the right panel, the relative error is compared against the smallest mesh, showing significant influence of refinement on solution quality in the interior, with flow around the clot remaining the same (shown on top of the error plot).

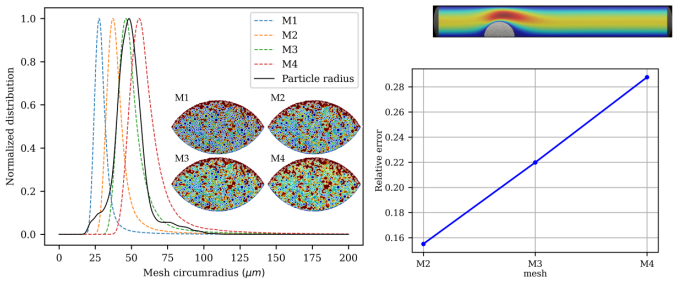

Fig. 3. Left: Pdf of the clot domain mesh element circumradii and the discrete particle radii, with flow solutions in inset. Right: Error relative to the finest mesh data in the clot domain. Relative error is defined as: $\int_{\Omega_T} |\underline{\mathbf{u}}_{M1} - \underline{\mathbf{u}}_i| / |\underline{\mathbf{u}}_{M1}| d\Omega$ where $i \in \{M2, M3, M4\}$.

References

[1] D. Mukherjee, and S. Shadden,"Modeling blood flow around a thrombus using a hybrid particle–continuum approach," Biomech. Model. Mechan., vol.17, pp.645–653, 2017.

[2] M. Alnæs, J. Blechta, J. Hake, A. Johansson, B. Kehlet, A. Logg, C. Richardson, J. Ring, M. Rognes and G. Wells, "The FEniCS Project Version 1.5," Arch. Num. Soft., vol.3, pp.9–23, 2015.

[3] A. Brooks, and T. Hughes, "Streamline upwind/Petrov-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations," Comput. Method Appl. M., vol.32, pp.199–259,1982.

[4] J. Anderson, P. J. Burns, D. Milroy, P. Ruprechet, T. Hauser, and H. Siegel, "Deploying RMACC Summit: An HPC Resource for the Rocky Mountain Region, " Proc. PEARC17, New Orleans, LA, USA, pp. 7, July 2017