Collaborative Research: Efficient Modeling of Incompressible Fluid Dynamics at Moderate Reynolds Numbers by Deconvolution LES Filters - Analysis and Applications to Hemodynamics

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ANNUAL REPORT – UNIVERSITY OF HOUSTON

May 16, 2017

Research and education activities

Students: 3 graduate students and 2 postdoctoral researchers have been involved in Year 1 of the grant.

- ◇ Graduate Students:
  - Kayla Bicol (F),
  - Krithika Rathinakumar (F),
  - Giuseppe Pitton (M).
- ◇ Postdoctoral Researcher:
  - Steffen Basting (M),
  - Yifan Wang (M).

Bicol participated in three conferences and Rathinakumar participated in two conferences. Bicol is the president of the Association of Women in Mathematics Student Chapter at UH. In the Summer 2017 Bicol will participate in the 23rd Industrial Mathematical & Statistical Modeling Workshop for Graduate Students at North Carolina State University. Basting graduated in October 2016 and has been offered a Research Associate position at TU Dortmund (Germany).

Research and education activities

- **Research Presentations:** Quaini presented the research related to this NSF proposal at over 15 conferences and seminars, which include: Plenary Talk at International Workshop on Fluid-Structure Interaction Problems (Singapore, May 30-June 03 2016), Invited talk at ECCOMAS 2016 (Greece, June 05-10 2016), Seminar at University of Zagreb (Croatia, June 17 2016), Invited talk at 2016 SIAM Conference on the Life Sciences (Boston, July 11-14, 2016), Invited talk at SIMAI 2016 (Italy, September 13-16, 2016), Colloquium Talk at Florida State University (Tallahassee, November 2, 2016), Colloquium Talk at Vanderbilt University (Nashville, January 17, 2017), Invited talk at SIAM CSE 2017 (Atlanta, February 27-March 3, 2017), Invited talk at Workshop on Applied and Computational Mathematics (Houston, March 9, 2017), Plenary Talk at 41st SIAM Southeastern Atlantic Section Conference, Florida State University (Tallahassee, March 18-19, 2017), Invited talk at International Conference on Finite Elements in Flow Problems 2017 (Italy, April 5-7, 2017).

Research and education activities

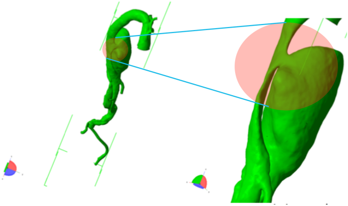
- **Courses for graduate and undergraduate students:** In the spring semester 2016 Quaini has taught Numerical Analysis for graduate students. In the fall semester 2016 Quaini has taught two sections of Linear Algebra with Matlab, and one section in the spring semester 2017. Topics of this project were mentioned as examples in this course to motivate the students.
- **Organization of Conferences:** Quaini co-organized with Dr. Olshanskii (UH) the Finite Element Rodeo on March 3-4, 2017. The Finite Element Rodeo is an annual, informal conference on finite element methods that rotates between several universities in Texas and Louisiana. Over 70 people participated in the conference, among them many students and post-docs.

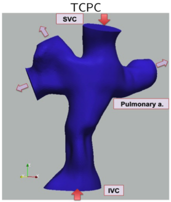
Research and education activities

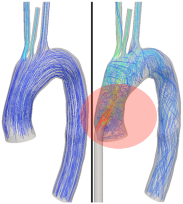
- **Organization of Mini-Symposia:** Topics from this project have been or will be presented at the following Mini-Symposia organized by Quaini: "LES modeling of turbulence: methods, analysis and applications" at SIAM CSE 2017 (Atlanta, February 27-March 3, 2017), "Fluid-Solid Interaction for Blood Flows" at FEF 2017 (Italy, 04/05-07/17), "Advanced Models and Methods in CFD" at Coupled Problems 2017 (Greece, 06/12-14/17), and "Advances in Reduced Basis techniques for flow problems in analysis, control, and optimization" at at the Sixth European Conference on Computational Mechanics (UK, 06/11-15/18).

Main motivation

- Blood flow can be highly disturbed, yet pulsatility prevents turbulence in general.
- In special cases (aortic flow, TCPC, LVAD, etc.) turbulence is observed.







In these cases, Large Eddie Simulation (LES) seems to be a good compromise between Direct Numerical Simulation (DNS, not affordable) and Reynolds-Averaged Navier-Stokes equations (RANS, not accurate).

Limitation of DNS

When $Re \gg 1$, energy is transferred from large eddies to smaller ones up to a characteristic scale, the so called Kolmogorov scale, where they are dissipated by viscous forces.

Kolmogorov scale: $\eta = Re^{-3/4} L$

A direct numerical simulation (DNS) aims at simulating all relevant scales up to the Kolmogorov scale. Therefore, the mesh size has to be $h \approx \eta$.

3D simulations: $\#Dofs \sim \left(\frac{L}{h}\right)^3 \sim Re^{9/4}$

The computational cost required by DNS becomes unaffordable for nowadays computers for *Re* greater than a few thousands.

Beyond DNS: Our Large Eddy Simulation approach

We choose to use filter stabilization techniques to model and extract the energy lost to resolved scales due to mesh under-refinement.
The idea is to filter the velocity obtained from the incompressible Navier-Stokes equations and use as end-of-step velocity a linear combination of the Navier-Stokes velocity and the filtered velocity.

We interpret these techniques as an **operator-splitting algorithm (EFR)**: At the time t^{n+1}

1. Evolve: Solve the incompressible Navier-Stokes equations and get $\mathbf{v}^{n+1}$, q^{n+1}.
2. Filter: $\mathbf{v}^{n+1} \rightarrow \overline{\mathbf{v}}^{n+1}$, with the associated $\overline{q}^{n+1}$.
3. Relax: $\mathbf{u}^{n+1} = (1-\chi)\mathbf{v}^{n+1} + \chi\overline{\mathbf{v}}^{n+1}$, $p^{n+1} = q^{n+1} + \alpha\chi\overline{q}^{n+1}$.

Step 2 has a key role: to tune the amount and location of eddy viscosity to the local flow structures.

Step 2: Filter

Given $\mathbf{v}^{n+1}$ from Step 1, find $\overline{\mathbf{v}}^{n+1}$:

$$\rho\frac{\overline{\mathbf{v}}^{n+1}}{\Delta t} - \nabla\cdot\left(2\rho\frac{\delta^2}{\Delta t}a(\mathbf{v}^{n+1})\nabla^s\overline{\mathbf{v}}^{n+1}\right) + \nabla\overline{q}^{n+1} = \rho\frac{\mathbf{v}^{n+1}}{\Delta t},$$
$$\nabla\cdot\overline{\mathbf{v}}^{n+1} = 0,$$

where

- $\delta = O(h)$ is a maximum filtering radius;
- $a(\mathbf{v}^{n+1}) \in (0,1]$ is the indicator function, with

$$a(\mathbf{v}^{n+1}) \simeq 0 \text{ in regions requiring no local filtering}$$
$$a(\mathbf{v}^{n+1}) \simeq 1 \text{ in regions requiring } O(\delta) \text{ local filtering;}$$

- $\overline{q}^{n+1}$ is the Lagrange multiplier for the incompressibility constraint.

The indicator function can be physical phenomenology -based. Such indicator functions are NOT based on rigorous mathematics, thus we preferred to use deconvolution based indicator functions.

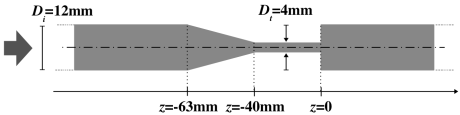
Note: this is a Stokes problem! Implementing this approach in a legacy Navier-Stokes solver does not require a big implementation effort.

Validation of our LES approach and novelties

Our LES approach was validated on an benchmark problem proposed by the U.S. Food and Drug Administration within the "Critical Path Initiative".

Goal of the initiative: to advance the application of CFD technology in the development and evaluation of medical devices.

Compare computational results with experimental data[1] for fluid flow in an idealized medical device with rigid boundaries.



Flow regimes: $Re_t = 3500, 5000$.

[Hariharan et al, *J Biomech Engrg* 2011] [Stewart et al, *CVET* 2012] [Stewart et al, *CVET* 2013]

[1] `https://fdacfd.nci.nih.gov/`

LES at $Re_t = 3500$

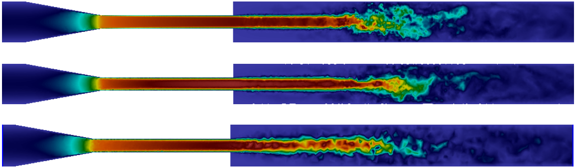
We considered several meshes:

mesh name	# nodes	# tetrahedra	Δt
$1200k$	2.3e5	1.2e6	1e-4
$900k$	1.8e5	9e5	1e-4
$330k$	6.5e4	3.3e5	2e-4
$140k$	3.1e4	1.4e5	3e-4

mesh $1200k$ — 240 s on 80 cores

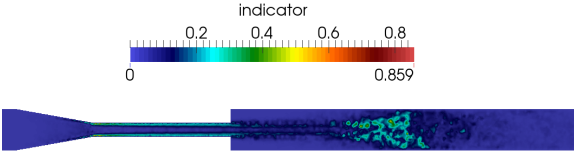
mesh $330k$ — 80 s on 48 cores

mesh $140k$ — 65 s on 16 cores

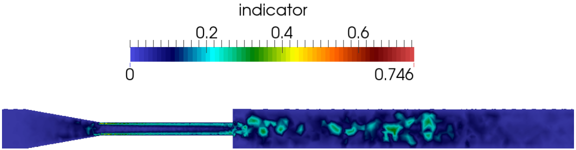


The results on mesh $1200k$ have been obtained with DNS, while the results with meshes $330k$ and $140k$ have been obtained with LES. With the coarser meshes, the finer details of the smaller turbulent structures are lost, yet thanks to the our algorithm the average behavior of the flow is well captured.

At $Re = 3500$, the indicator function obtained with mesh $330k$ takes the largest values where the jets breaks down:



whereas with mesh $140k$ the indicator function takes fairly large values all along the jet:

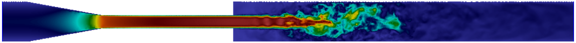


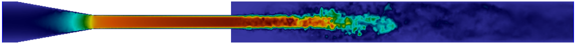
The numerical results obtained with both meshes are in good agreement with the experimental data.

LES at $\mathrm{Re}_t = 5000$

We considered several meshes:

mesh name	# nodes	# tetrahedra	Δt
$3000k$	5.5e5	3e6	1e-4
$1900k$	3.7e5	1.9e6	1e-4
$900k$	1.8e5	9e5	1e-4
$330k$	6.5e4	3.3e5	2e-4

mesh $3000k$  280 s on 208 cores

mesh $900k$  220 s on 96 cores

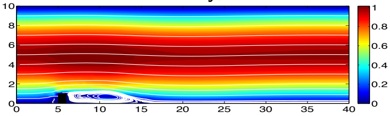
Despite the large number of nodes and tetrahedra, mesh $3000k$ is not refined enough for a DNS to give results in good agreement with the experimental data. We had to use LES with all the meshes and obtained results in good agreement with the experimental data. A paper with all the results obtained with LES has been published in the Int. J. Numer. Meth. Fluids in 2016.

Sensitivity to the filtering radius

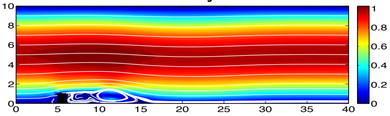
One critical aspect of filter stabilization techniques for the Large Eddy Simulation of incompressible flows at moderately large Reynolds number (in the range of few thousands) is the selection of the filter radius δ. This drives the effective regularization of the filtering procedure,and its selection is a trade-off between stability (the larger, the better) and accuracy (the smaller, the better). We investigated the sensitivity of the solutions given by our approach to the filter radius by introducing the sensitivity systems, analyzing them at the continuous and discrete levels, and numerically testing on two benchmark problems. We showed that the velocity sensitivity magnitude correctly identifies the region of the domain where the velocity is sensitive to variations of δ. Moreover, we showed that the our approach correctly predicts the physical solution for different values of δ, and is much less sensitive to the parameter choice than the classical Leray model. One paper containing our preliminary work on this has been accepted in the Springer-ECCOMAS series "Computational Methods in Applied Sciences".

We considered the two dimensional channel flow past a forward-backward step. The correct physical behavior of the solution is a smooth velocity profile, with eddies forming and detaching behind the step. The solutions given by the classical Leray model are similar away from the step, but behind the step they exhibit very different behavior: for $\delta = 0.25$ there is no eddy separation, while for $\delta = 0.1$ the correct transient behavior of eddy shedding is predicted.

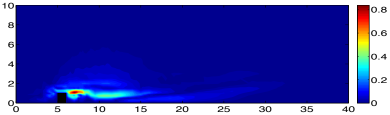
Classical Leray, $\delta = 0.25$



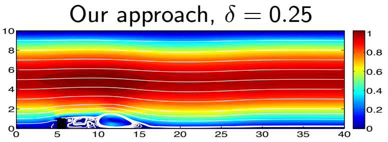
Classical Leray, $\delta = 0.1$

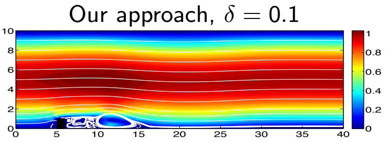


This sensitivity to δ near the step and lack of sensitivity away from the step are predicted in the plot of the velocity sensitivity magnitude for $\delta = 0.25$.

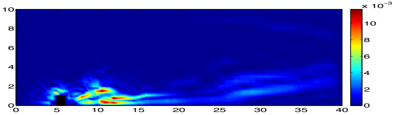


The same test was run with our approach. We observe that both solutions correctly predict eddy shedding behind the step.





Moreover, we observe that the velocity sensitivity magnitude for $\delta = 0.25$ is quite small. In fact even though it is largest behind the step, just as in the classical Leray case, for our approach the sensitivity magnitude is almost 2 orders of magnitude smaller.



Hence our approach correctly predicts the physical behavior with both choices of δ, and is much less sensitive to the parameter choice than the classical Leray model.

Open-source library

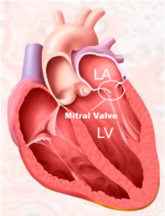
All the computational results have been performed with LifeV[2], an open-source library of algorithms and data structures for the numerical solution of partial differential equations with high-performance computing techniques. Life V includes solvers for incompressible fluid dynamics, structural problems, and fluid-structure interaction. Life V is written in C++ and is entirely coded with an Object Oriented approach and advanced programming features. Life V was successfully installed on clusters called Maxwell and Opuntia at the UH Center for Advanced Computing & Data System, and on several clusters of the XSEDE consortium.

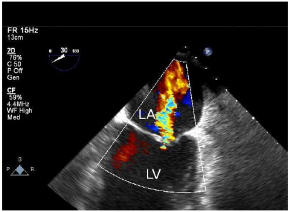
An important outcome of this work is that the code created for it is incorporated in an open-source library and therefore is readily shared with the community.

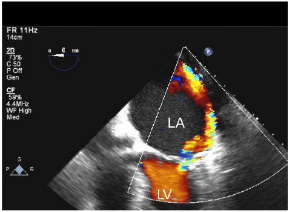
[2] `http://www.lifev.org`

LES for Coanda effect in cardiology

Mitral valve Regurgitation (MR) is a valvular heart disease which is associated with the abnormal leaking of blood from the left ventricle (LV) into the left atrium (LA) of the heart. Accurate estimation of regurgitant volume, especially in the case of wall-hugging jets, known as Coanda effect.



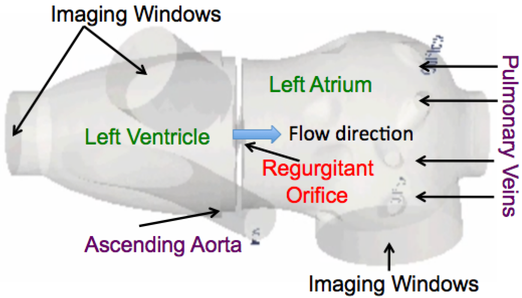




Understanding the flow conditions, and the size of the leaky orifice for which Coanda effect occurs, is one of the biggest challenges of modern echocardiography.

Mock Heart Chamber

A pulsatile flow loop was designed by our collaborators at the Methodist Hospital to model in vitro the hemodynamics conditions encountered in patients with MR. The loop incorporates an anatomically “correct” Mock Heart Imaging Chamber.

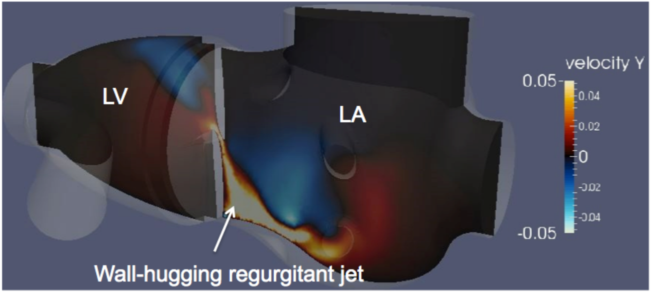


Until now, it was not possible to reproduce Coanda effect *in vitro* in an imaging chamber. The goal is to understand the flow conditions and orifice geometries lead to the Coanda effect *in vitro*.

Simulation of Coanda effect in mock heart chamber

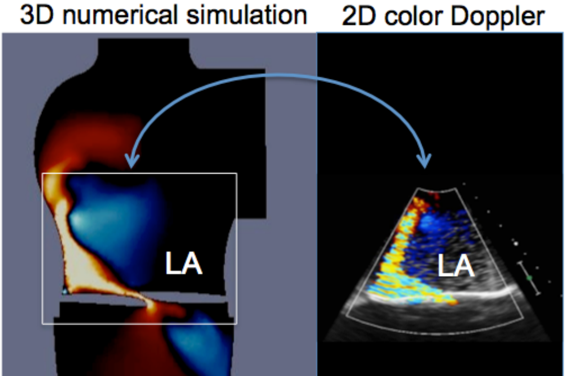
With post-doctoral associate Yifan Wang, we performed 3D simulations of regurgitant flow in the realistic mock heart chamber for a range of Reynolds numbers, including Re $= 3000$, which corresponds to the realistic regurgitant mitral valve flow. The wall hugging jet (Coanda effect) was observed only at higher Reynolds numbers, and for slender regurgitant orifices. One paper on the simulations of the Coanda effect in mock heart chamber has been accepted for publication in Cardiovascular Engineering and Technology.

3D MOCK HEART CHAMBER



Comparison with 2D color Doppler image

3D simulations of eccentric regurgitant flow were compared with 2D color Doppler image of the same flow in the mock heart chamber. Excellent agreement was achieved. The picture below shows a 2D slice of our 3D simulation (left) and a 2D color Doppler image of the same flow (right). Blue corresponds to backward flow (from top to bottom), while red corresponds to forward flow (bottom to top). A strong wall-hugging regurgitant jet can be observed in both pictures.

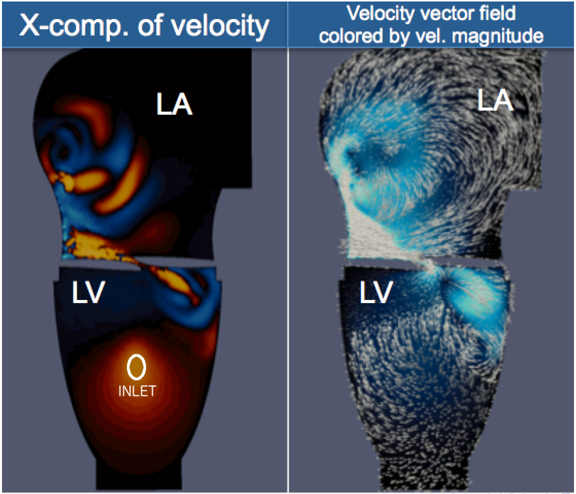


3D Visualization of flow

Our 3D flow simulations for the first time reveal that the regurgitant jet is actually spiraling away from the orifice. A vortex is generated downstream from the orifice, which in 3D generates **vortex rolls**. See Figures on the next page. The vortex rolls push the regurgitant jet even closer to the wall. The spiraling motion of the jet gives rise to the regions of flow that are orthogonal to the imaging source, and would be seen as regions with zero velocity. Due to the low velocity there, as well as on the vortex side, the jet appears smaller than it actually is, giving rise to the under estimation of the regurgitant volume based on the jet appearance on an echocardiographic image.

The figure in the next slide shows the x-component of velocity (left), and the velocity magnitude, together with the velocity vector field (right). The x-component of velocity is toward the viewer. Blue denotes velocity moving away from the viewer, while red denotes velocity moving toward the viewer.

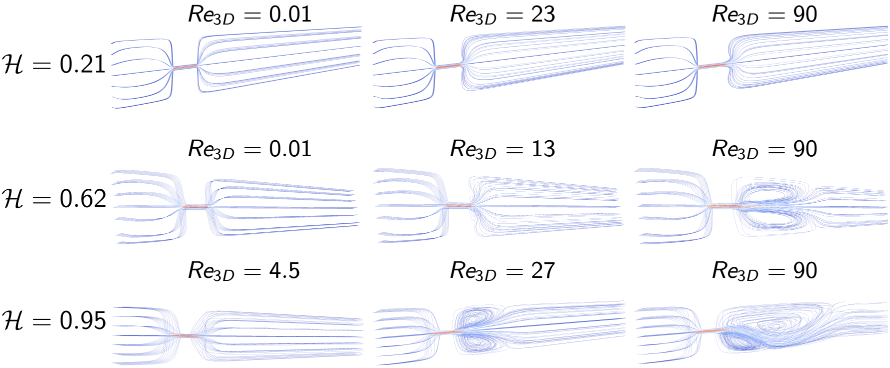
One can see that there is a thin blue region located between the jet and the wall, indicating entrainment of particles associated with Coanda effect. On both sides of the jet there are regions of velocity that are orthogonal to the jet motion, making the jet smaller in appearance on an echocardiographic image.



Preliminary results with Reduced Order Modeling

In order to further reduce the computational costs associated with flow simulations, we considered **Reduced Order Modeling** (ROM) techniques. We start by applying standard reduced order methods (e.g., Reduced Basis and/or Proper Orthogonal Decomposition) to the simulation low Reynolds number flow. This is a preliminary step, necessary to understand the capabilities of ROM methods before applying them to high Reynolds number flow. In particular, we focused on the hydrodynamic stability of solutions of the incompressible Navier-Stokes equations for a Newtonian and viscous fluid in 3D. Our preliminary work shows that standard reduced order methods allow to capture complex physical and mathematical phenomena, such as bifurcations in the parametrized Navier-Stokes equations, at a fraction of the computational cost required by full order order methods. One manuscript reporting on these results has accepted for publication in the Journal of Computational Physics.

We considered a 3D contraction-expansion channel with fixed aspect ratio $\lambda = 15.4$. We let the normalized channel depth $\mathcal{H}$ (with $\mathcal{H} = 1$ corresponding to the 2D channel) and the Reynolds number vary.



We see that at low values of $\mathcal{H}$ the symmetry breaking bifurcation is pushed to higher values of Re_{3D} due the vertical walls.
The computational time for one simulation with full oder model is 240 CPU hours and with the reduced order model is few seconds.

Fluid-structure interaction with a DG-ALE approach

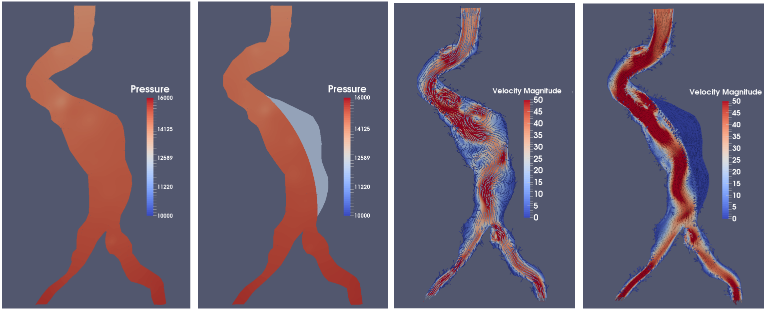
In many cardiovascular applications, blood (modeled as an incompressible, viscous, and Newtonian fluid) interacts with an elastic/viscoelastic structure such as cardiovascular tissue or vascular prosthesis. We proposed a numerical approach based on a high-order discontinuous Galerkin (with Interior Penalty) method, combined with the Arbitrary Lagrangian-Eulerian approach to deal with the motion of the fluid domain, which is not known a priori. The proposed numerical approach provides sharp resolution of jump discontinuities in the pressure and normal stress across fluid-structure and structure-structure interfaces.

The proposed numerical method has been tested on a series of benchmark problems, and has been applied to a fluid-structure interaction problem describing the flow of blood in a patient-specific aortic abdominal aneurysm (AAA) before and after the insertion of a prosthesis known as stent-graft. The stent-graft excludes the aneurysm sack from circulation and lowers the probability of AAA rupture. One paper on this work has been submitted to the Journal of Scientific Computing.

AAA before and after stent-graft

The figures below show the computed pressure p without and with stent-graft (SG) and the computed velocity magnitude $||\mathbf{u}||$ and vector field without and with stent-graft at roughly 1/3 of the cardiac cycle:

p without SG p with SG $||\mathbf{u}||$ without SG $||\mathbf{u}||$ with SG



The proposed DG method provides a sharp resolution of the pressure jump that occurs across the stent graft. We see that after the stent graft implantation the vortices are inhibited and confined, and the pressure exerted onto the aneurysm sack walls is reduced.

Plans for the Next Reporting Period

- Complete the benchmarking of our LES approach up to Reynolds number 6500, which is comparable with the largest Reynolds number in the human circulation system.
- Perform the sensitivity analysis for the deconvolution order, which is a key parameter in the indicator function.
- Perform MRI imaging of flow in Imaging Heart Chamber and compare the results with numerical simulations (3D computations validation phase).
- Perform further 3D numerical simulations with pulsatile flow conditions to further understand the flow conditions and orifice shapes that lead to Coanda effect.
- Improve our ROM approach by using Centroidal Voronoi Tessellation to obtain "smarter" bases.
- Extend the ROM approach to higher Reynolds numbers.