Research, education activities, and findings for the project on Coanda effect

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• Graduate and Undergraduate Students: Four graduate students (Martina Bukac, Sibusiso Mabuza, Steffen Basting, Luca Bertagna) and two undergraduate student (Kayla Bicol and Thomas Scott) were involved in the project. In addition to the research performed by Martina Bukac, she participated in three conferences and two workshops: Workshop for Young Researchers in Mathematical Biology (MBI Ohio, September 2011) and Frontiers in Mathematical Biology Young Investigators Conference (University of Maryland, March 2012). One of those conferences took place at the NSF funded Mathematical Biosciences Institute. Bukac was mentored by both Canic and Quaini. She graduated with a PhD in May 2012. Bukac was offered a post-doctoral position at the University of Pittsburg, Department of Mathematics, with a starting date of August 2012. She was then offered a Tenure Track position at the University of Notre Dame in May 2014, which she accepted. Mabuza graduated in May 2013. He was offered a postdoctoral position at the University of South Africa. He is expecting an offer from Sandia Labs, where he would like to go as a postdoc.

• **Conference Presentations:** Canic presented the research related to this NSF proposal at over 30 conferences and seminars, which include: the Keck seminar (Rice University, November 11), 3 invited lectures at the SIAM PDE meeting (San Diego, November 2011), Mathematics Colloquium (UC Irvine, January 12), NSF-NIH Math Biology meeting (University of Maryland, March 2012), Midwest Numerical Analysis Conference (University of Notre Dame, May 12), HYP2012 (an international meeting on Hyperbolic Conservation Laws, Padova, Italy, June 2012), MoST 2012 (an International Workshop on Transport Problems, Moseille Valley, Germany, July 2012), ECCOMAS 2012 (European Congress on Computional Methods in Applied Sciences and Engineering, Vienna, September 10-14, 2012), Distinguished Rockwell Lecture at the University of Iowa (October 3, 2012), Colloquium at the University of Michigan (November 2, 2012), Hosted Steffen Busting (November 19-23, 2012), Colloquium at Tulane University (January 25, 2012), Colloquium at the University of Pittsburgh (February 22, 2013), Lecture at the regional AMS meeting in Ames, Iowa (April 27, 2013).

 Presentations: Quaini presented the research related to this NSF proposal at over 20 conferences and seminars, which include: Graduate Student Seminar (University of Houston, October 2011), Numerical Analysis Seminar (University of Maryland, October 2011), Mathematics Colloquium (Rice University, November 11), Scientific Computation and Numerical Analysis Seminar (Rice University, March 2012), Seminar at the Department of Biomedical Engineering (Georgia Tech, May 2012 and February 2014), Invited presentation at the University of Jyvaskyla, (Finland, June 18-19, 2012), MATHICSE Seminar at EPFL, Switzerland (June 12, 2012), 2012 SIAM Annual Meeting, Invited Minisymposium Talk (Minneapolis, June 19, 2012), ECCOMAS 2012, Invited Session Presentation (Vienna, Austria, Sept 10-14, 2012), MPF2013 (Italy, June 10-14 2013), 2013 SIAM Annual Meeting, Invited Minisymposium Talk (San Diego, June 19, 2012), USNCCM13, Invited Minisymposium Talk (Raleigh, July 22-25, 2013), Invited presentation at MBI (Columbus, October 28-31 2013), Scientific computing seminar at Emory University (Atlanta, April 2, 2014).

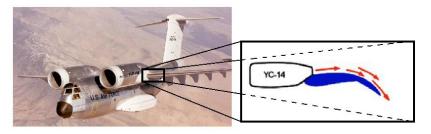
- **Collaboration with Medical Specialists:** Collaboration with Dr. Stephen Little MD of Methodist Hospital, Houston, was established. Experimental laboratory at the Methodist Hospital was used to validate the flow conditions studied in this project (see pictures below).
- Organization of Symposia and Workshops: The PIs organized a Special Topics Workshop at MBI in October 2013. The title of the Workshop was "Mathematics Guiding Bioartificial Heart Valve Design". Invited Speakers included: Prof. Arash Kheradavar of UC Irvine, Prof. Boyce Griffith of NYU Medical Center, Dr. Stephen Little of Methodist Hospital, Prof. Alessandro Veneziani of Emory University, and the PIs. The PI (Canic) was the main organizer of the SIAM PDE conference in San Diego, December 2013.
- **Special Courses:** Canic taught a <u>Mathematical Hemodynamics</u> course in the Fall of 2011. Topics of this project were mentioned as examples in that course.

Background: The Coanda effect in aerodynamics

The COANDA EFFECT is the tendency of a fluid jet to be attracted to a nearby surface.

It is named after Romanian aerodynamics pioneer Henri Coanda (patent 1934).



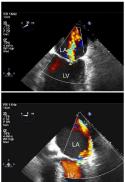


The YC-14 uses the Coanda effect to increase the lift for a short take off and landing.

The 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 into the left atrium of the heart. MR jets can undergo the Coanda effect.

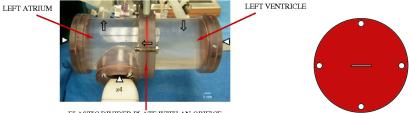




One of the biggest challenges in echocardiographic assessment of MR is to estimate the severity of mitral valve regurgitation when blood flow jet through the leaky mitral valve undergoes Coanda effect. Understanding the flow conditions, and the size of the leaky orifice for which Coanda effect occurs, is one of the biggest challenges of modern echocardiography.

Research highlights: Mock heart chamber

A pulsatile flow loop was designed at the Methodist Hospital to model in vitro the hemodynamics conditions encountered in patients with MR in order to assess Doppler derived estimates with measurements. [Little et al., *Ultrasound in Med. & Biol.* 2008]



ELASTIC DIVIDER PLATE WITH AN ORIFICE

Our collaborators* have never been able to reproduce the Coanda effect in the imaging chamber.

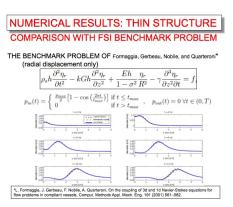
*S. Little MD, S. Igo MD, W. Zoghbi MD (Methodist Hospital) and Dr.

C. Hartley (Baylor College of Medicine)

Research highlights: Computational Scheme 2D

 \bullet To study the flow conditions associated with valve regurgitation, we

have been working on the design of novel fluid-structure interaction solvers that are particularly suitable for studying FSI involving heart valves, or cardiovascular tissue in general. We designed a novel partitioned, loosely coupled scheme, called the kinematically-coupled β -scheme, whose simimplementation. ple modularity, unconditional

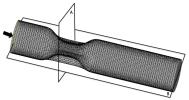


stability, and low computational costs, make it particularly appealing for solving FSI problems in hemodynamics. The figure above shows excellent comparison of our scheme and a monolithic scheme on a FSI benchmark problem in 2D.

Computational Scheme 3D

• Further developments of this scheme to study realistic problems in 3D, and FSI with heart valves is under way. The figures below show the application of the scheme to a FSI problem defined on a realistic 3D problem modeling coronary artery stenosis.

Computational mesh and stenotic geometry.

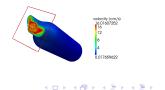


Pressure and velocity vector field.





Velocity at the stenotic throat.

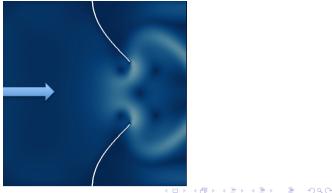


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Computational Scheme: Valve Problem

• We are extending the kinematically-coupled β scheme to a benchmark problem with heart valves. A modification of the Arbitraty Lagrangian -Eulerian (ALE) method, based on level-set & front tracking, is being implemented to deal with the deficiencies associated with ALE approaches applied to problems with large structural displacements, associated with heart valves.

Our simulation of a FSI computational benchmark problem for heart valves in 2D.



The novel loosely-coupled partitioned scheme: Summary

• Our simulations indicate that the kinematically-coupled β scheme, which is based on the time-discretization via Lie operator splitting, is particularly suitable for the use in multi-physics problems involving biofluidics.

• This novel scheme has been now implemented and used for the numerical simulations of several problems in hemodynamics, including: FSI between an incompressible fluid and a thin structure, modeled as Koiter shell/membrane, both linear and nonlinear models were used, FSI with a thick structure modeled by the equations of 2D/3D linear elasticity, FSI with composite structures, such as the arterial walls of human arteries, FSI with thin structures treated with cardiovascular devices called stents, etc.

• This class of schemes has now been used not only by the PIs and their collaborators, but has now found widespread use by several different authors, applied to different multi-physics applications involving incompressible, viscous fluids and structures with comparable densities.

• Various novel results were found, related the to biomedical application at hand, thanks to the use of this scheme.

The novel loosely-coupled partitioned scheme: Education activities

Graduate student Martina Bukac was the primary developer of the loosely-coupled partitioned scheme for FSI between blood flow and arterial walls. Bukac graduated in May 2012 and was hired as a Post-doctoral Fellow in the Department of Mathematics, and the University of Pittsburgh. She received a Tenure-Track Assistant Professorship offer at the University of Notre Dame in May 2014.
Graduate student Steffen Basting has been involved in the development of the kinematically-coupled β scheme, in combination with the front-tracking/level-set method to study FSI involving heart valves. Basting is a graduate student at the University of Erlangen, Germany.

Basting visited UH for 2 extended visits to work on the research funded by this grant.

• Seven peer-reviewed publications resulted so far from this research, and 11 conference/seminar presentations were given by the PIs on the topic of this research.

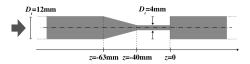
Research Highlights: Continued

• Existence of a solution to a fluid-structure interaction problem in blood flow was established using, in the main steps of the proof, the loosely-coupled numerical scheme, mentioned above. This work was obtained together with post-doctoral associate Dr. Boris Muha. This work shows, among other things, that the kinematically-coupled scheme converges to a weak solution of a benchmark non-linear fluid-structure interaction problem in blood flow. One publication appeared in the Archive for Rational Mechanics and Analysis, one in the Journal of Differential Equations, and 2 have been submitted.

• An advection-diffusion solver in moving domains was generated to study particle transport and diffusion in blood flow, modeling the use of nano-particles in cancer drug delivery, enhanced by an ultrasound excitation of the motion of arterial walls. The fluid-structure solver, mentioned above, is used to provide the underlying pulsatile blood flow conditions in human arteries. This is a work in progress with graduate student Sibusiso Mabuza. One publication was submitted, and two are near completion. Mabuza graduated with a PhD in May 2014.

Validation against experimental measurements - part I

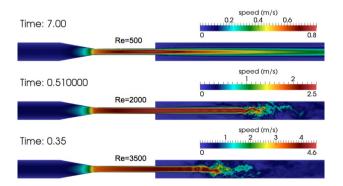
• Validation of our solver in fixed domains: the FDA nozzle **benchmark problem.** We developed a monolithic solver for FSI in hemodynamics, based on the work related to the PhD thesis of Annalisa Quaini. This algorithm was validated on an FDA-benchmark problem "Computational Fluid Dynamics: An FDA's Critical Path Initiative. https://fdacfd.nci.nih.gov/." See also Hariharan P, et al.. Multilaboratory Particle Image Velocimetry analysis of the FDA benchmark nozzle model to support validation of Computational Fluid Dynamcis simulations. J. Biomech. Engrg. 2011; 133:041 002. Excellent comparison for a large range of Reynolds numbers was obtained. One publication in the International Journal for Numerical Methods in Biomedical Engineering and two conference papers on this work appeared in 2013.



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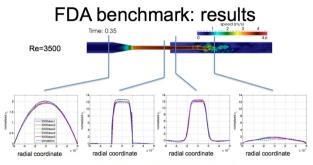
Research Highlights

FDA Benchmark: Results



The FDA benchmark considers flow in a nozzle for different Reynolds numbers spanning the laminar (top figure), transitional (middle figure), and turbulent regimes (bottom figure).

Research Highlights



COMPARISON WITH MEASUREMENTS

- · Normalized axial velocity as a function of the radial coordinate
 - Slight underestimation of axial speed in the throat
 - Accuracy in the recirculation zones downstream the throat

All the results up to Reynolds number 3500 were obtained using Direct Numerical Simulations (DNS) and showed excellent agreement with the PIV measurements acquired by the FDA laboratories.

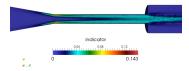
Higher Reynolds numbers

Direct numerical simulation (DNS) has a major limitation: high computational costs due to the huge number of degrees of freedom needed to fully resolve the flow features.

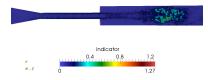
An alternative to DNS is to use filter stabilization techniques to model and extract the energy lost to resolved scales due to mesh under-resolution. The idea is to filter the velocity obtained from the incompressible Navier-Stokes equations and use as end-of-step velocity a linear combination of the Navier-Stokes velocity and the filtered velocity. The role of the filter is to tune the amount and location of eddy viscosity to the local flow structures. This is done through an indicator function which takes values close to zero where no local filtering is needed and close to one where filtering is required. 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.

The indicator function

At Re = 500, the indicator function takes its largest values in the boundary layer:



At Re = 3500, the indicator function is still different from zero in the boundary layer, but now it takes the largest values where the jets breaks down.



This work has been done in collaborations with Prof. A. Veneziani and PhD student L. Bertagna from Emory University. Two articles are in preparation.

Validation against experimental measurements - part II

• Validation of our solver in moving domains: A moving orifice problem. Our monolithic fluid-structure interaction algorithm was validated against experimental measurements performed in a heart flow chamber with a moving orifice simulating a regurgitant mitral valve. Two publications resulted from this research: one in Cardiovascular Engineering and Technology, and the other one in the Journal of Biomechanics.

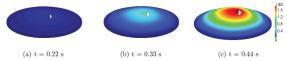
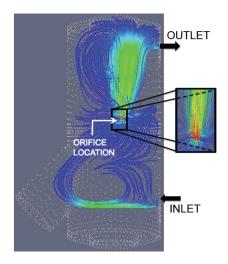


Figure 7: Structure displacement at time (a) t = 0.22 s, (b) t = 0.33 s, and (c) t = 0.44 s for experiment 3. The legend shows displacement magnitude in mm.

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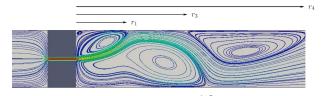
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Research Highlights



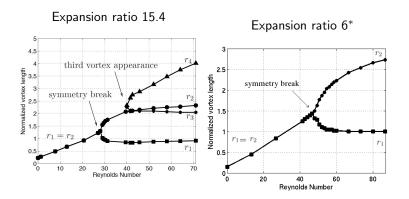
Research Highlights

•Bifurcation diagram describing transition to Coanda effect: flow through a contraction-expansion channel was studied. A bifurcation diagram was obtained, indicating the parameters for which the Coanda effect is generated. This bifurcation diagram depicted in the next slide, shows the transition from symmetric to asymmetric flow through a pitchfork bifurcation. The asymmetric flow has the property of hugging the walls of the receiving chamber, exhibiting the Coanda effect as shown in the figure below. The flow regimes associated with the Coanda effect were studied, and used later in this project, to recreate the Coanda effect in a stylized regurgitant valve problem. One manuscript was submitted to the Journal of Fluid Mechanics, reporting on the results of this research.



Re = 71.3

Bifurcation diagrams



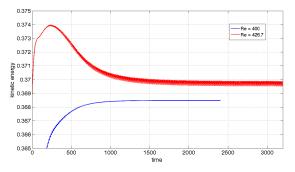
The critical Reynolds for the symmetry break reduces when increasing the expansion ratio.

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The Hopf Bifurcation

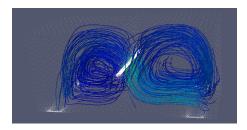
• Transition to Hopf Bifurcation: At Re = 426.7, the asymmetric solution experiencing Coanda effect, loses its stability and a one-parameter family of periodic solutions bifurcates from the stationary solution. This phenomenon is known as Hopf bifurcation. We are the first group which was able to clearly capture the transition to Hopf bifurcation for the flow in the contraction-expansion channel. Results of this research were reported in the manuscript submitted for publication to the Journal of Fluid Mechanics.



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3D chamber - streamlines at Re = 100

• By using the results reported above, we were able to recreate Coanda effect in a 3D chamber with a fixed orifice, mimicking the heart chamber with a regurgitant valve. Only elongated orifices, and not the circular ones, can produce Coanda effect, for flow conditions corresponding to the Reynolds number which is larger than the critical pitchfork bifurcation Reynolds number.

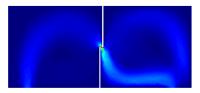


Elongated uneven orifice

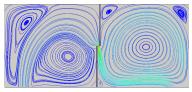
Research Highlights

• The corresponding 2D slices of the 3D simulations, mentioned above, are shown below, clearly indicating the wall hugging jet known as Coanda effect. The influence of this flow condition on the ultrasound detection of mitral valve regurgitation and its severity can now be studied *in vitro*, using the mock heart chamber. The bifurcation analysis indicates that *only the regurgitant mitral valves for which the regurgitant orifice occurs along almost the entire coaptation zone of the valve*, produce the Coanda effect. This is important information from the imaging prospective because detection of severity of mitral valve regurgitation in this case should be performed at the angles aligned with the long axis of the valve, producing realistic regurgitant volume estimates.

Uneven orifice 3D (section)



Uneven orifice 2D



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Coanda Effect in Patient Specific Geometries

• To translate our Coanda effect mathematical results from the *in vitro*. stylized geometries and controlled flow conditions into patient-specific geometries, we initiated a collaboration with a scientific computing group at Emory University, led by Prof. Alessandro Veneziani. One of the pressing issues is image recon-A slice through a patient specific struction from patient-specific geometry of left ventricular output CT images, of the complex getract with valve ometries involving human heart valves. The patient-specific data AORTIC ROOT are obtained from our collabora-CROSS-SECTION tors at the Methodist DeBakey Heart and Vascular Center. The AORTIC VALVE figure on the right shows an LOCATION example of a coarse computa-I FFT VENTRICULAR tional mesh associated with such OUTPUT TRACT CROSS-SECTION a geometry. The next step is to perform flow simulations and Netgen 5.1 compare them with experimental data.

Parallelization and open-source Framework

• In 2012-2013 a parallel version of our solvers was developed and merged with an Open-Source library of parallel solvers LifeV (http://www.lifev.org/home). 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 a cluster called Xanadu at the Texas Learning and Computation Center, on a cluster called Maxwell at the UH Research Computing Center, and on several clusters of the XSEDE consortium. Parallelization enabled us to perform the FDA-benchmark problem of flow through a nozzle and simulations of the Coanda effect in patient-specific geometries.

Summary

Our research produced so far 22 research articles, 2 book chapters, and 1 peer-reviewed conference proceedings. Two classes of computational schemes (monolithic and partitioned) were developed to study FSI involving incompressible, viscous fluids and elastic/viscoelastic structures, and a computational scheme to study reactive transport in moving domains was developed. Our computational solvers are currently being made available to the general public through an Open Source parallel library of solvers called Life V (http://www.lifev.org/home). Additionally, over 50 talks at conferences, colloquia talks and research seminars were presented. One special course on Mathematical Hemodynamics was taught in the Mathematics Department at the University of Houston. Three lectures for high-school students were presented. Four graduate, two undergraduate students, and two post-docs have been involved in this project. Two graduate students graduated with a PhD (Bukac, Mabuza) and two are expected to graduate in 2015 (Basting, Bertagna).

A collaboration with medical specialists at the Methodist Hospital in Houston was established, where a heart flow chamber designed with the help of the numerical simulations provided from this research was designed. This is now enabling a novel in vitro study of mitral valve regurgitation (MR) and its detection using ultrasound imaging modalities. The mathematical bifurcation diagram helped design a flow chamber which recreates the flow conditions in patients with mitral valve regurgitation exhibiting Coanda effect, which is notoriously difficult to resolve using ultrasound technologies for assessment of severity of mitral valve regurgitation. The mathematical bifurcation diagram showed, among other things, that the mitral valve regurgitation in patients with Coanda effect, must occur along the entire coaptation zone of the valve, and not at an isolated point. Based on these finding, we hypothesize that ultrasound imaging of MR in such patients should be performed along the long-axis of the valve, whenever possible, which would increase the accuracy of the assessment of the severity of mitral valve regurgitation. Experimental study of this hypothesis is currently under investigation at the Methodis DeBakey Heart and Valve Center.