Chair for Computational Analysis of Technical Systems

RWTH AACHEN UNIVERSITY

Prof. Marek Behr, Ph.D.

Lehrstuhl CATS Schinkelstr. 2 52062 Aachen

Schinkelstr. 2
52062 Aachen
GERMANY
Telefon: +49 241 80-999 01
Fax: +49 241 80-999 10

behr@cats.rwth-aachen.de

Biuro Dziekana
Izabela Herman
Wydział Inżynierii Środowiska i Energetyki
ul. Konarskiego 18
44-100 Gliwice
POLAND

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Referee report for the dissertation of Mr. Aleksander Sinek, submitted to the Department of Environmental Engineering, Mining and Energy of the Silesian University of Technology titled:

Integration of Statistical Data Analysis and Surrogate Modeling for Uncertainty Quantification, Sensitivity Analysis and Inverse Problems Involving Fluid-Structure Interaction Models

Motivation and Goals

Simulation of fluid flow problems is a relatively new method of analysis, complementing long-standing experimental and analytical approaches. As such, the simulation techniques are continually being extended to new areas of applications, where computational analysis is yet to make a full impact. One such broad area is bioengineering; in comparison to hydro- or aeronautical engineering, simulation approaches have been much slower to take hold there. The major reason is that the components to be analyzed—whether tissues or bio-fluids—are orders of magnitude more complex in comparison with relatively simple constitution of fluids like water or gases like air. They are in general micro-structured, composed of a large variety of micro- and mesoscale constituents, like cells or proteins, which lead to a micro-scale behavior that is extremely difficult to characterize concisely.

The particular case of blood flow is important in a variety of bioengineering contexts, from performance of mechanical heart-assist devices (blood pumps) and artificial heart valves for long-term therapy, to design of oxygenators for emergency use, to mass production of dialysis equipment. Although the description of the blood as a fluid can be simplified to that of Newtonian fluid and treated with standard simulation software for many applications, one needs to consider the non-Newtonian aspects for many applications.

An even more challenging aspect present in nearly all bioengineering applications is the fluid-structure interaction (FSI). The fluid-filled domain itself is unknown in such problems, and the necessity to track this domain has given rise to many different approaches. Interface-tracking methods adapt the mesh – by deforming it – in order to always match the mesh and fluid boundaries. Interface-capturing is a robust alternative, which, however, if used without care, can lead to slowly converging, i.e., relatively inaccurate, results. Moreover, the multiple physical phenomena needs to be coupled, and solved together in an efficient and general way.

Thesis Organization

The thesis is organized in eight chapters plus a summary, bibliography, and appendices.

Chapter 1 describes concisely the motivation of this work. The need for non-invasive yet accurate measurement of arterial stiffness as precursor to cardiovascular intervention planning is clearly stated. An ultra-sound-based procedure is postulated and the necessary development steps listed. The challenges involved in repeated model-based simulations comprising the inverse problems are pointed out. A statistical analysis is identified as a critical ingredient that is necessary for the proposed procedure to have a real-life impact. The main ingredient of this computational approach is an FSI model. Two avenues towards obtaining such a model are proposed, to be pursued in parallel. Further, some basic approaches to FSI are outlined, followed by an introduction to reduced-order modeling, uncertainty quantification, and inverse problems. The topic of surrogate models receives much more attention compared to the other topics, and one wonders if some of the material here should not be moved, e.g., Chapter 3. Finally, the chapter includes the outline of the thesis that follows.

Chapter 2 devotes ca. 20 pages to image processing and filtering, and statistical data analysis including detailed discussion of statistical regression and variance. Then, on only two pages, the FSI governing equations including both fluid and solid mechanics are introduced. This is not the weighting I would have assigned to these topics, but it is (barely) sufficient for later discussion of FSI issues.

Chapter 3 is about surrogate modeling (again), uncertainty quantification (UQ), and Bayesian inference. The discussion starts with sampling techniques, from random through Latin hypercube, to Halton and Hammersley. They are not fully explained, but well described and illustrated. The next section is about Gaussian process regression (GPR); I was hoping to learn about this topic, but the way the section is written, it is unlikely to be understood by someone not already thoroughly familiar with the subject; it might have been better to cite references instead. Next, non-intrusive model reduction is considered. Finally, UQ and Bayesian statistics are described.

In Chapter 4, the major contribution of this thesis – an experiment for testing the inverse problem based on FSI – is designed. It is a flow chamber which offers control over volume and pulsatility of cardiovascular-like flow, and allows optical observation of the response of elastic tube, meant as arterial phantom. High-speed cameras generate images in two perpendicular frames, which are then processed to quantify the lateral displacement of the arterial wall, while the flow and pressure in the mock loop are also monitored. The statistical tools from Chapter 2 are applied to extract maximum information from a possibly biased pressure and flow measurements, eliminating for example temporal drift over multiple pulsatile cycles. Phantoms are then subjected to uniaxial tensile tests to obtain their material properties – aspects that will be later the target of clinical analysis, if the approach is successful. This externally obtained data is not discussed extensively, but it appears to have large uncertainty.

As the second necessary ingredient of the inverse problem, the FSI simulation is set up. This is done first with ANSYS CFX fluid solver, which also offers FSI option based on deforming mesh approach. Some mesh refinement study is performed, although this strikes me as inadequate. Changing mesh from 117 to 440 thousand fluid elements is hardly enough to assess mesh independence; this does not even correspond to doubling the spatial resolution. In any case, since ANSYS did not prove to be robust with respect to material properties, another attempt was made using a different solver called FEBio. A satisfactory agreement was demonstrated in the end between phantom and numerical displacements, as long as large-displacement structural model was employed.

The statistical approach and reduced order model is shown in Chapter 5. The FSI system is parametrized, e.g., accounting for variability of pulsatile flow curves. Then this parameter space is mapped using GPR. It is not clearly stated but it appears that this was not entirely successful, suffering from large memory footprint and overfitting. Nevertheless, it provided a suitable reduced model, and performed better than reduced-basis alternative. Finally, the full FSI model was subjected to UQ, to identify the most critical parameters that affect the stiffness measurements.

Chapter 6 offers the conclusions and directions for future research. It is followed by a bibliography with nearly 200 entries, and summaries of the thesis in English and Polish.

Conclusion

The main contribution of the thesis was already pointed out above: Novel concept for in vivo measurement of arterial stiffness based on inverse computational problem combined with the numerical model of fluid-structure dynamic interaction. The approach developed certainly has a great potential for improving on the currently prevalent measures of arterial degradation, and thus for significantly contributing to the accuracy of future clinical decisions.

The material in this English-language thesis is logically arranged and almost ready for publication; some suggestions for improvement have been included at the end of this review.

The work can be in principle considered for awarding a distinction ("wyróżnienie"). For it speaks the unusual combination of computational, experimental, and statistical expertise amply demonstrated by the thesis. The topic is also of utmost importance and the societal motivation for this research is very clear. On the negative side is a limited number of resulting publications (so far). I feel that the question of distinction can be better answered after the upcoming defense. I recommend without reservations that the document be accepted as a dissertation by the Silesian University of Technology.

Aachen, January 3, 2025

Univ.-Prof. Marek Behr, Ph.D.

Minor remarks and corrections to the thesis of Aleksander Sinek:

- Title of the thesis and some section titles are oddly capitalized. Either use "title case" with all major words capitalized or do not capitalize at all.
- Throughout, "i.e.," and "e.g.," should be used (with commas).
- Page 2: Meaning of "regional" is typically opposite of "global"; in this context, "global" would be more appropriate.
- Page 3: "increases the inaccuracy" → "lowers the accuracy".
- Page 4: "ultrasound" misspelled. Use spell-checking throughout.
- Page 6: Statement that "FEA is a general framework for analyzing solid dynamics" is clearly wrong. FEM and thus FEA is a discretization approach not tied to a particular application. It is being used not only for solid mechanics but for countless other PDE-based models, including CFD (cf. ANSYS Polyflow or Altair AcuSolve, and even employed FEBio). Please use "computational structural mechanics" or something similar when referring to the structural side of the FSI problem.
- Page 6: "as described" is misspelled. Further misspellings will not be pointed out.
- Page 6: We see sometimes "FEBio" and sometimes "FEBIO".
- Page 7: "FSI" is written "FSi". All such instances should be caught when spell-checking.
- Page 9: "Starting of with" → "Starting off with" or "Starting with".
- Page 10: Should we understand that, e.g., only 17 articles on Gaussian process regression in engineering were found in recent literature? Maybe limitations of this literature study should be more clearly stated.
- Page 11: The way citations are included is not consistent, e.g., [38,43][55]-[58] should be [38,43,55-58]. This should be automatic in LaTeX with an appropriate package.
- Page 24 and rest of the chapter: Inconsistent notation – X vs. x – and capitalization.
- Page 49: Indexing for gradient components starts with 0? What is N?
- Page 50: At least B, C, and E tensors could be defined here, as opposed to trace operator that is self-explanatory.
- Page 55: "This two key" → "These two key". Capitalization continues to be ad hoc.
- Page 57: Equation (3.3) uses symbols of which none were introduced.
- Page 58: Multiple misspellings on this page.
- Page 59: What is F in equation (3.8)?
- Page 61: Are kernels and covariance functions used interchangeably? Both K and k are used on this page and it's not clear why.
- Page 62: Not sure what the vertical axes represent here, notation is mysterious.
- Page 64: What are the colors in Figures 3.3 and 3.4?
- Page 94: First circle in Figure 4.7 could be drawn more accurately.
- Page 106: Figures 4.15 through 4.17 should be moved closer to where they are referred to.
- Page 108: Figure 4.20 is referred to before 4.19.
- Page 109: Again FEA is used incorrectly as a shorthand notation for solid mechanics.
- Page 109: "steady" is a wrong term here, maybe "insensitive to mesh refinement".
- Page 119: Is pressure "P" or "p"? What is the point of "Pshift"? What are "Pi"'s?
- Page 125: What is "f.ex."?