Workshop Scientific Report

Please do not repeat the program (unless there were last-minute changes) or the initial description - we already have this material.

Title	TREND IN COMPUTATIONAL HEMODYNAMICS
Organizers	Simone Melchionna Alfio Quarteroni Efthimios Kaxiras

Scope of the workshop (one-two paragraphs)

In the last few years, computational hemodynamics has been witnessing a growing interest with the goal of better understanding blood circulation in model and physiological conditions. Blood and the vascular system constitute a multi-faceted environment composed of several physical layers with fundamental implications in biomedical sciences. The scope of the workshop was to bring together the viewpoints and perspective from scientists involved in the study of hemodynamics and physiological fluid flows. Besides the physical modelling, the workshop aimed at addressing topics related to the fluid mechanics, bio-chemical and medical levels of hemodynamics, with focus on common cardiovascular diseases, such as atherosclerosis.

One crucial aspect of the workshop was to assess the most appropriate computational frameworks to tackle blood micro- and macro-circulation. Given the large diversity of scenarios, from capillaries to large coronary arteries, there is large demand for computational methods to be both accurate and efficent. A correct understanding of blood flows requires the inclusion of vascular deformability, physiologically correct inflow and outflow conditions, and physiologically motivated models to emulate the systemic nature of the cardiovascular system. The workshop also aimed at providing a perspective in the development of highly efficient softwares for hemodynamics on conventional parallel CPUs or accelerator-based hardware. The critical assessment of methodologies in handling large-scale vascular flows with or without red blood cells was intended to be discussed during the workshop.

Main **outcomes** of key presentations (one page)

The presentations had several outcomes, some of them related to cardiovascular diseases and the design of medical devices. As a general introduction, C. Feldman provided a bird-eye view on cardiovascular diseases and the factors that influence atherogenesis and plaque evolution. His talk was particularly relevant as it addressed the measurements of atherosclerosis with both IVUS and CT scanners, together with the biological implications in the endothelium region. The biological and biomechanical implications on blood flow and the reshaping of the endothelium were discusses. S. Weinbaum described the several aspects of glycocalyx and its implications as a porous material for the fluid flow pattern with the ensuing intramural fluxes. The skying-capabilities of red blood cells were discussed together with the consequences on shear-stress transduction. Several talks concerned the available computational approaches to micro and macrocirculation.
Regarding the usage of novel methologies to handle complex scenarios, J.-F. Gerbeau described methods to derived medical data and optimize their inclusion via proper variational and filtering techniques. Another important topic was related to fluid-structure interactions and the use of proper modelling of cardiac valves. L. Formaggia expounded his studies on fluid-structure interactions and with 0, 1,and 3-dimensional closures to represent complete cardiovascular systems. N. Stergiopoulos presented methods and models for the one-dimensional representations of complete arterial trees, together with the medical and patient-specific implications of this systemic representation. J. Moore described the biomechanical interaction of stents with the artery wall from both the fluid mechanics and solid mechanics points of view. B. Chopard presented his studies on aneurisms, handled via a modification of the Lattice Boltzmann method. J. Latt described a numerical method to handle fluid-structure interactions in effective terms. R. Nash described the on-going activity at Imperial College about creating an infrasctructure along the Virtual Physiology project and its connections with hemodynamics while F. Milde described the studies on angiogenesis, as it is carried on at ETH in Zurich, an activity that requires to intervene at modeling level to study the implications of vascularization. A few talks raised the important aspect of investigating situations of medical relevance, as for example in studying different types of stenting, in reproducing the behavior of implantable devices for cardiac assistance, or the effects of aneurisms, plaques and valves.
When dealing with red blood cells and circulation, several topics were covered. At experimental level, H. Stone provided data on complex cell/fluid interactions, such as the flow of red blood cells and the formation of bacterial biofilms. One important aspect concerned the shear-induced release of ATP from red blood cells and the mechanism of ATP release as the cell deforms, the next topic being about the formation of thread-like structures of biofilm.
At computational level, G. Karniadakis presented several computational approaches to blood flow simulations, including two different ways to include red blood cells. Interesting results on red blood cells aggregation were presented and the high-performance sides of his approach. D. Poulikakos described his studies in understanding the celebrospinal liquid, a different physiological fluid but yet related in some respect to hemodynamics. L. Munn described an approach to modeling red and white blood cells as used in the study of angiogenesis. The ensuing imaging of vessel structure and function as related to tumor growth were presented.
S. Melchionna presented a novel approach to handle blood flows inclusive of red blood cells by a combination of the Lattice Boltzmann method and Molecular Dynamics, a technique specifically designed to handle large-scale vascular flows. G. Gompper discussed his studies on microcirculation by looking at the motion of vesicles and red blood cells, cell reshaping and tank treading motion. C. Misbah presented the several theoretical issues related to a correct description of red blood cells, regarding the vesicular face of cell motion and more red blood cell-specific aspects.

Report on selected discussions (one page)

eg. Were there interesting hints for new research? for new developments? for collaborations?

During the workshop there was no session dedicated to a round table but each talk was given enough time (45 minutes per speaker) to allow for questions on specific topics.

The majority of speakers were computational scientists who tackle hemodynamics and biofluids in diverse ways. The first block of talks were broad in scope and raised several issues on the most appropriate approaches to model biofluids, for hemodynamics, cerebral fluids or angiogenesis. The traditional CFD techniques, either the conventional Navier-Stokes level or the more mesoscale level, can only be employed on three-dimensional geometries where an accurate dataset is available on human or animal vascular geometries. The implications with the difficulties encountered by the imaging methodologies (CT, IVUS, MRI) are apparent and the accuracy of the numerical techniques need to overcome the accuracy on the reconstructed morphologies. As pointed out in some talks, this is often not the case and a good deal of smoothing on the experimental data is needed in order to provide sufficient numerical stability and physical realism. In some circumstances not only the geometry can be extracted from actual measurements but, as was made clear, informations about compliances can be reconstructed. This is highly valuable in view of the upsurge of methods and approaches for fluid-structure studies.

Another crucial missing information regards the systemic nature of the circulatory system. In this respect, several talks and discussion raised points on how to model the peripheral system with sufficient accuracy and how to possibly include the periphery with one-dimensional or zero-dimensional closures (alike the well-known Windkessel closure). This issues pointed towards the missing information on flowrates and pressure drops on extended vascular networks.

Regarding fluid-structure interactions, at least two approaches were underlined during the workshop, a first more complete way to include the tissues via extended elasto-mechanics representations or a more succint approach where the tissues were represented as effective membranes. The two approaches are rather different in spirit, the first one being typically eulerian, more accurate and also more cpu-demanding, while the second is typically lagrangian, based on lumped parameters and more lightweight.

Similar differences in spirit were seen in the presentations and discussions on blood at red blood cells level. As Karniadakis pointed out, a model should serve a specific purpose and, in the realm of hemodynamics, several different scientific aspects are targeted, ranging from circulation in capillaries and in microdevices, to the large scale coronary arteries and the aorta. Again, several methodologies were presented and discussed during the question time, including Molecular Dynamics, Multi-Scale Dynamics, Dissipative Particle Dynamics and Multi-Particle Collision Dynamics. All these methods cope well with the inclusion of solutes in flow conditions and provide a more flexible environment than conventional Navier-Stokes solvers. In fact, the role of these mesoscale methods is typically to cover different space/length scales by reproducing the single red blood cell behavior. For instance, several talks reported on reproducing complex non-linear response of blood, such as the Faraheus-Lindqvist effect, by using effective bottom-up models. Some sophisticated models can also reproduce red blood cell reshaping and elastomechanic response in narrow capillaries at the expense of the computational efficiency.

The several reports described in some talks on complex biomechanical behavior, like the complex ATP-red blood cell interplay or the role of leukocytes in complete blood flows, pose new challenges to the computational community, in particualr in designing multi-scale numerical methods that can cover wider length and space scales without sacrifying accuracy.

In conclusion, the workshop served for the several groups represented in the workshop to have a direct confrontation on blood dynamics. Several topics with transversal, yet fundamental, implications were touched upon, high-performance computing on traditional or novel hardware, ranging from BlueGene to GPU architectures, being an example. Given the above range of topics, the workshop has been successful in bringing together the diversified community working on hemodynamics. This was a rare and precious occasion as the mathematical, physical, engineering and medical groups rarely meet in international meetings. Some collaborations were initiated between the attendees, and more than anything else, the workshop served as a collective confrontation point.

To what extent were the **objectives** of the workshop achieved (strong points, weak points)? (one paragraph at least)

Being hemodynamics in the end a rather focused field, the talks and ensuing discussions achieved the objectives of providing a broad view on this field to the non-experts together with technical accounts on specific research from well-established groups. This was the dual objective of the workshop and several scientists who attended the meeting, working in hemodynamics or different fields, such as biology or neuroscience, provided positive feedbacks to the organizers.
Probably for the first time, a specific effort was made to bring together top-down and bottom-up approaches to hemodyamics. The effort was rewarded by the fact that in many circumstances the range of applications of bottom-up routes reached the macroscale realm but demanded for a more systemic account of the circulatory system, as much as the more macroscopic approaches demand for a local representation of blood based on its basic constituents. The weak point of the workshop was to having scarcely homogenized approaches to blood circulation. As the community includes scientists and methodologies from different backgrounds and educations (experimental, theoretical and computational, from mathematics, physics and engineering), it is not obvious that a common language and common objectives are identified. Nonetheless, the strong points outperformed the weak points and the workshop achieved its main objectives.

Do you have suggestions for new workshops/tutorials/conferences on the topic?

Given the success of the first workshop on hemodynamics organized by Cecam (with more than 45 attendees), and given that many computational groups working on computationtal hemodynamics are related to Cecam, the topic deserves a follow-up in the forthcoming years. The strategic implications together with the social and medical impact of hemodynamics is worth to pursue the organization of this type of events, as much as investigating broader aspects of biofluidics and its implications to biology and physiology.
On general grounds, Cecam can provide a stable meeting place for the computational community involved in biology and physiology, a community that is witnessing a rapid growth in recent years.