

Human-scale vascular simulation with HemeLB - Progress towards the virtual human

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1. Background

The ambition of creating a virtual human - a simulation model encompassing the individual physiological characteristics of a single person - remains a significant ongoing challenge for scientific, computational and medical researchers and practitioners. The realization of a virtual human would permit a variety of treatment options to be assessed and the best option for the wellbeing of the individual be selected. The continuing advance in the capability and capacity of both desktop and high-performance computing platforms means that achieving this goal is closer than ever. Taking advantage of this computational performance demands simulation frameworks that can scale efficiently to large-scale systems whilst still resolving the essential physics and physical characteristics of the individual. The coupling of separate codes for simulating physiological systems separated by both function and scale will also be necessary to underpin the development of a full virtual human.

In this presentation we will discuss some of our recent progress in developing the HemeLB blood flow simulation code as a candidate for simulating the vasculature of the virtual human. In particular, we will highlight the execution characteristics of the code that demonstrate that it can already operate at the forefront of simulation performance on some of the fastest computers on the planet. We will also present our strategy for a lightweight incorporation of elastic wall effects into HemeLB and our framework for coupling HemeLB with the Alya Red heart model for the simulation of a full cardiovascular.

2. Methodology

The open-source HemeLB code [1, 2] has been developed with a specific focus on the study of three-dimensional vascular flows at high-resolution and at extreme scales. This is enabled through the use of the lattice Boltzmann method (LBM), an alternative approach to solving the Navier-Stokes equations for fluid flow with more traditional finite element or volume approaches. The localised computational kernel of the LBM permits two particular advantages for blood flow simulation. The first is that it is a straightforward algorithm to parallelise leading to good computational performance on both small and large computational scales. The second is that it enables complex geometric shapes to be accommodated using local assignment of the simulation site to its particular category - e.g. fluid, wall, inlet, outlet. We take advantage of this characteristic to provide a candidate for a simple representation of elastic walls. HemeLB has been specifically optimised to enable efficient performance on the sparse geometries that are characteristic of vascular domains.

To facilitate coupling of HemeLB, we have developed a strategy for the transfer of boundary

data to and from a simulation whilst attempting to minimise the amount of data needing to be exchanged [3, 4]. To enable the simultaneous study of both arteries and veins, we have employed this framework to couple two separate instances of HemeLB and have demonstrated this with examples of human-scale veins. The representation of the capillary beds between the two simulations is represented by the coupling framework. To further couple HemeLB to the Alya Red heart model, we have extended this methodology to include the transfer flow information between the boundary interfaces of the two simulations.

3. Results

In collaboration with the POP Centre of Excellence, we conducted a performance analysis of HemeLB on SuperMUC-NG – one of the fastest computers in the world. This study simulated flow through a geometry of the circle of Willis vascular structure consisting of over 10 billion lattice sites. Here it was demonstrated that HemeLB could scale strongly up to the full production partition of SuperMUC-NG consisting of almost 310,000 CPU cores [3]. Equipping this version of the code with the self-coupling strategy was then used to demonstrate strong scaling of the coupled framework to 96,000 CPU cores [4]. These results (see Figure 1) demonstrate that HemeLB already has the capacity to effectively run simulations of the scale necessary for the virtual human.

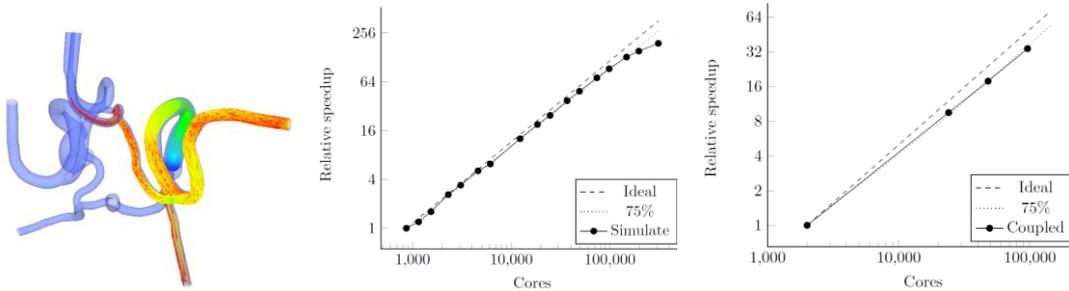


Figure 1 Performance of HemeLB on SuperMUC-NG using a 10 billion site geometry of a circle of Willis (left). Single instance performance (centre) demonstrates strong scaling to the full production partition of almost 310,000 CPU cores whilst the self-coupled implementation (right) demonstrated strong scaling to 96,000 CPU cores.

In a recent case study, we have utilised our self-coupled framework to simulate blood flow in the arteries and veins of the left forearm [4]. This was conducted in the context of creating an arteriovenous fistula between the radial artery and cephalic vein. This is a procedure conducted in patients with kidney failure to provide an access point for dialysis to take place. Our study highlights the impact of individual physiological conditions can have on blood flow through the vasculature and emphasises the need for cooperation between modellers and clinicians to advance the capabilities of virtual human simulation. In Figure 2 we illustrate the vessels studied in this example, the changes in blood flow generated through the creation of a fistula and the detailed flow visualisations that can be obtained when 3D solvers are used to study such flow problems.

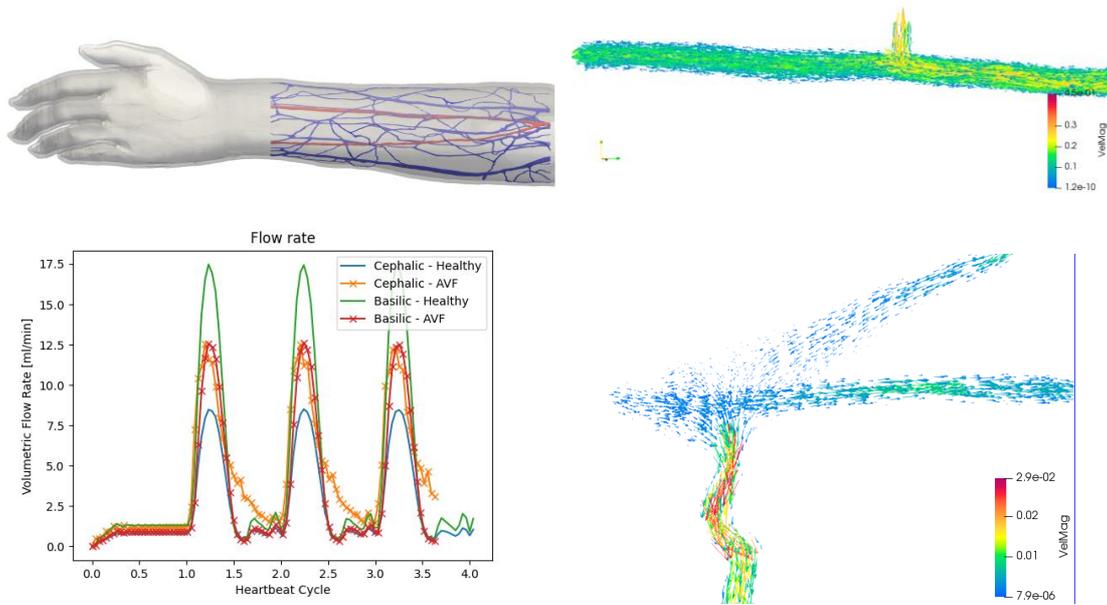


Figure 2 A set of individualised arteries and veins from the left forearm (top-left) were utilised to study blood flow through them before and after the creation of an arteriovenous fistula. In a post-maturation state, the presence of the fistula caused significant changes to the volume of blood flowing through key veins (bottom-left). A key advantage of 3D simulations is the ability to generate detailed images of flow through complex geometries as illustrated here for arteries (top-right) and veins (bottom-right) from the fistula system, both are represented by velocity vectors coloured by velocity magnitude in m/s.

Typically, the simulation of blood vessels with elastic walls demands the coupling of a fluid flow solver to a solid mechanics solver. This procedure can become prohibitively expensive when the simulated domain is on the human-scale. Indeed, within the scientific literature, there is debate on whether rigid walls are sufficient for large blood flow simulations or an explicit coupling is necessary [5]. Our lightweight wall model represents a compromise between these two positions by capturing key features of flow through elastic walled cylinders whilst still adhering to the LBM’s principle of local collision computation.

Our coupling of HemeLB and Alya Red represents a proof of concept of how our coupling strategy can permit multiple monolithic codes to effectively communicate with each other for the purpose of blood flow modelling. We demonstrate how the combination of Alya Red with the self-coupled implementation of HemeLB will enable the full circulation of systemic blood flow to occur on a human-scale set of arteries, veins and ventricles.

4. Summary

In this presentation, we have highlighted several advances made in our efforts for simulating blood flow in the virtual human with HemeLB. These, along with the code’s large-scale performance characteristics, demonstrate that we are progressing well along the pathway to enabling such simulations to become more routine, especially in future clinical settings. However, many hurdles remain before such a situation can arise. Examples of these pertain to data preparation, management and storage, visualisation of results, reliability of simulation execution and the spread of accelerator technology in high-performance computing.

5. References

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