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A LATTICE BOLTZMANN MODELING OF BLOODFLOW IN CEREBRAL ANEURYSMS

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Abstract. *We present numerical simulations of bloodflow in cerebral aneurysms, obtained with the open source software Palabos which provides a flexible, highly parallelized and publicly available environment for the lattice Boltzmann (LB) method. LB models are promising tools for biomedical modeling that compares well with more traditional CFD techniques and can be easily augmented to include non-Newtonian rheology or biological processes. In this paper we shall discuss a LB model describing the formation of a thrombus in a cerebral aneurysmal cavity, whether spontaneous or induced by a flow diverter (stent).*

1 INTRODUCTION

Numerical simulations have become a very promising component to open new avenues in biomedical research. For instance, they provide a better understanding, at the system level, by combining several processes, often at different spatial and temporal scales in the same "in-silico" experiment. In addition, they may provide clinicians with a new decision support tool for diagnosis and treatment planning.

As an example, the modeling of restenosis in stented arteries[1, 2] has been studied recently using a multiscale simulation approach based on the so-called Complex Automata (CxA) framework[3, 4]. In this approach different sub-processes (bloodflow, growth of smooth muscle cells, thrombus formation and drug diffusion) are represented as lattice Boltzmann, cellular automata or particle based models and coupled across the scales.

The lattice Boltzmann (LB) and Cellular Automata (CA) approaches[5, 6] offer a mesoscopic abstraction of a physical or biological process in term of the interaction of fictitious particles or cells, interacting on a discrete space-time universe. CA and LB models comply with the CxA framework and can be coupled in a generic way[3, 4] in order to build a multiscale simulation out of flexible and reusable software components.

In this paper we are interested in the modeling of thrombosis in cerebral aneurysms. Our goal is to develop the numerical tools to implement, in patient-specific geometries, the basic thrombosis model proposed by ourselves in[7, 8, 9].

In section 2 we shall recall the main ingredients of the thrombosis model and the results we have obtained so far. Next, in section 3 we present the Palabos LB framework that we keep developing to perform 3D massively parallel simulations in a biomedical context. Finally, we compare in section 4 the Palabos LB solver with simulations done with ANSYS, a well-known commercial flow solver.

2 THROMBOSIS IN CEREBRAL ANEURYSMS

Cerebral aneurysms are undesired local deformations of the wall of a brain vessel whose rupture can be lethal. The natural repair of an aneurysm is through a thrombosis process that fills in the cavity, eventually leading to the remodeling of the wall vessel. It is now well accepted that the blood flow pattern in the aneurysm cavity plays a crucial role in the evolution of the disease[10].

In order to induce thrombosis in the cavity one has modify the flow pattern in an appropriate way. For instance a clot can be induced by coiling the aneurysm or, also, by deploying a flow diverter stent (also called flow modulator) in the parent vessel, across the aneurysm neck. The effect of the flow diverter is to modify the blood flow pattern in the aneurysmal cavity, thus creating favourable conditions for the thrombosis to start. It is observed that the clot induced by different flow diverters may have quite different morphology and stability. Some clots may re-dissolve and re-canalization (i.e. reformation of a lumen in the aneurysmal cavity) occurs after a while. If an aneurysm is at risk of rupture, an appropriate medical intervention is required. Flow diverters stents are a non-

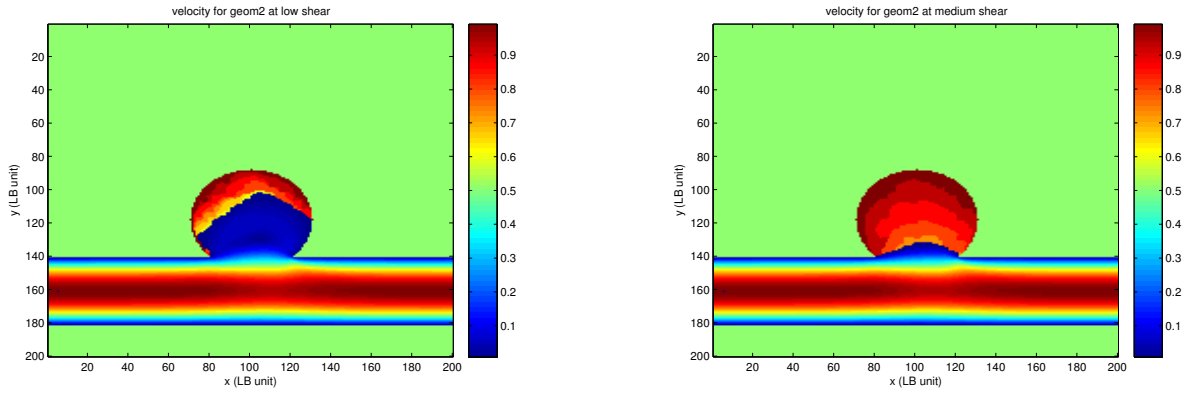

Figure 1: Simulation of the thrombus formation in a side-wall aneurysms. On the left, the shear stress threshold controlling the thrombus growth is rather small and the clot process stops early (partial clotting). On the right, the threshold is higher and the clot is almost total. Note in both images the structure of the clot as a succession of layers.

invasive treatment and can be quite successful, provided they induce the right type of clot inside the cavity.

In order to model such a process and eventually to provide recommendations on which stent design is most appropriate for a given patient, we have proposed a mixed LB and CA approach[7, 8, 9]. This model considers a LB model for the blood (whether Newtonian or not) coupled with a CA model for the transport of platelets and red blood cells and a CA aggregation model to mimic thrombus growth.

In short, this intra-aneurysm clotting model is based on several assumptions, all of them supported by qualitative biological observations. The model postulates the existence of a shear stress threshold below which thrombosis initiates in the aneurysm and above which thrombosis stops. The model also includes a probability of adhesion of platelets to the wall, as a function of the shear stress. The lower the shear stress the higher the adhesion probability. In addition, the thrombus growth process is modeled through a aggregation probability and reaction time.

To the best of our knowledge this model is currently the most promising one to describe how thrombosis occludes the aneurysm cavity: it has reproduced several features observed in giant aneurysms for which no explanations were known before (existence of either partial or full clotting, onion-skin structure of the clot, threshold in the value of the aneurysm aspect ratio). As an illustration, fig. 1 shows the simulated formation of the clot in a side-wall aneurysms, with different values of the shear-stress threshold. As the cavity occludes, the flow pattern changes, because of the new boundary conditions. During this process, the shear stress increases and, according to the threshold values, thrombosis may stop before filling up the cavity.

These simulations are 2D and performed under simple flow conditions and simple geometries. In order to study patient specific geometries together with real stents, one needs

to develop more advance software tools. They are discussed in section 3.

Note that this model is based on postulated values of thresholds and parameters that need to be calibrated. In a recently submitted European VPH project, we propose a set of laboratory experiments that will allows us to extract the correct values of these parameters and to assess the validity of the model at a mesoscopic level.

3 LATTICE BOLTZMANN SIMULATIONS WITH PALABOS

In this section we discuss the lattice Boltzmann (LB) Palabos software upon which we are extending the 2D thrombosis model presented in the previous section. We assume that the reader is familiar with the LB method in itself and we refer those who are not to standard reviews or textbook (see for instance [5, 6, 11]).

Although traditional flow solvers have been successfully used to simulate flows in cerebral aneurysms[10], the LB approach, being closer to physics than to mathematics is well suited to combine mechanical processes (hemodynamics) with biological ones (thrombosis processes) in an intuitive way. Due to its mesoscopic level of description the LB method allows a rule-based modeling approach, quite appropriate to represent stiff and non-linear aggregation process, controlled by the flow properties. In addition LB calculations scale very well on massively parallel hardwares and their implementation on GPUs have turned quite successful[12], offering a potential for unprecedented fast simulations.

The Palabos environment (http://www.lbmethod.org/palabos) is a free, open-source software that implements many features of the LB methods in a very flexible and reusable way. It keeps improving over time and is now used by an increasingly large community of users. In addition, Palabos is compatible with the CxA coupling methodology discussed in section 1. That makes this software quite appropriate to address multiscale simulations.

Our goal here is not to present the detailed architecture of Palabos, nor to give a description of how to program an application. We refer the reader to the website for such questions. Instead, we want to list a few important capabilities of this platform, especially in the context of blood flow simulations for patient specific geometries.

The Palabos platform proposes an efficient data-structure which allows parallelisms and grid refinement, even for complex geometries. This data-structure is called "multi-block". Each block contains a Cartesian mesh, with possibly different spatial and temporal resolution. The computational domain is covered by such blocks, whose sizes are automatically determined according to the shape of the domain. This decomposition is completely transparent for the user who only needs to import the desired computational domain. For instance, fig. 2 show the case of a synthetic aneurysm geometry, with one inlet and two outlets. This domain is initially specified by its surface, then it is transformed into a voxel-based geometry and then partitioned into several blocks in order to save as much memory as possible. The consistency of the coordinate system across the block is guaranteed by their hierarchical construct. At the largest scale, a unique block covers the bounding box of the object. This block is then iteratively divided and only the parts that cover the domain are kept. It is only at the lowest scale that the LB mesh is

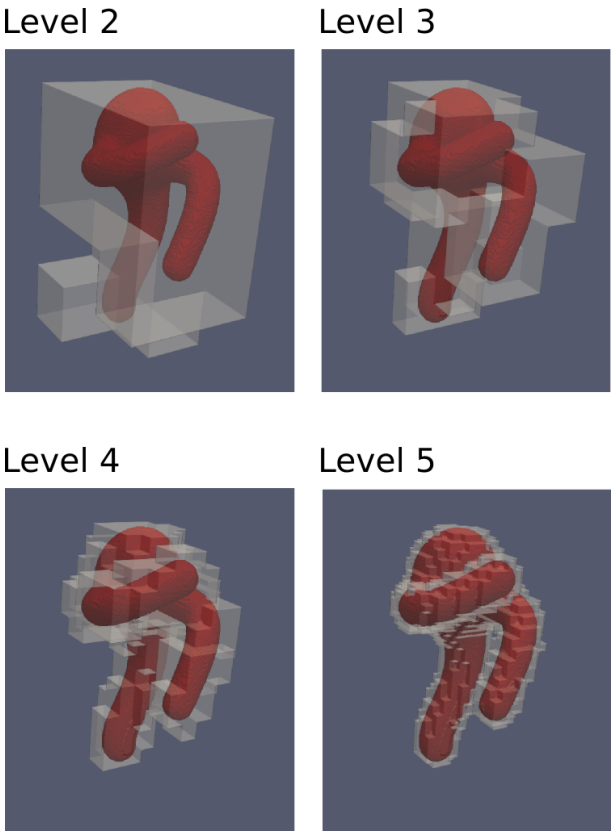

Figure 2: Example of the multiblock data-structure used in Palabos. The construction of the final block structure is based on a hierarchical process of refinement and is shown in the lower right panel.

instantiated.

In addition to saving memory with irregular computational domains, the multiblock approach allows for parallelism and grid refinement. Each block can be associated to a different processor and has its own grid resolutions. Adjacent blocks are automatically coupled through inter-processor communications if needed and/or with scale interpolation in case of grid refinement. The 3D grid refinement will be released soon in the public version of Palabos.

In Palabos, one can easily switch among different collision operators. The BGK, MRT and regularized[5, 13] collisions are already implemented. Similarly, several standard on-lattice boundary conditions are available. For instance a Womersley velocity profile can be imposed in the outlet whereas wind-kessel pressure boundary conditions are used for the outlets. Similarly, any physiologic flow condition can be implemented. Fig. 3 shows a snapshot of the velocity streamlines for a pulsatile simulation. Palabos is interfaced with Paraview, which makes visualization easy.

For several biomedical applications, it is necessary to compute the Wall Shear Stress (WSS) as this quantity affects the behavior of the biological cells at the vessel wall. Also,

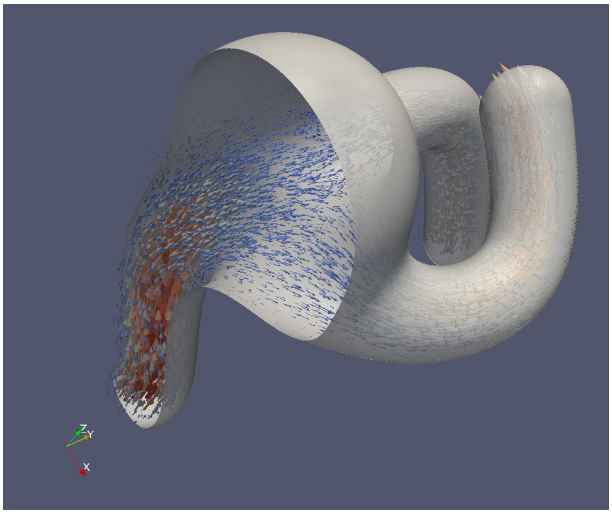

Figure 3: Snapshot of the velocity field in our synthetic cerebral aneurysm.

as discussed in section 2, the dynamics of the clot formation process depends on the WSS. Palabos implements a way to obtain the WSS. Note that WSS in LB simulations can be computed to satisfactory accuracy even for voxel-based boundary conditions[14]. Another important question in bloodflow simulation is whether one can be satisfied with a Newtonian rheology or not. Palabos implements the Carreau-Yasuda rheology[15, 16], using standard parameters for the blood. Fig. 4 shows the value of the WSS on the aneurysm sac, for the Newtonian and non-Newtonian rheology. Noticing that the scales in both cases are not the same, we can observe the clear difference between the two rheology. In view of the thrombosis model of section 2, the right rheology may impact very much the existence and the volume of the final clot.

4 BENCHMARK

There have been several comparisons between LB and classical CFD solvers[17, 18] in terms of accuracy and CPU performance. Although the LB method is a much more recent approach, it performs usually very well, especially for complex flows in complex geometries. More specifically, for a biomedical problem, Axner et al[19] have demonstrated that both approaches give the same quality of results without however discussing the CPU efforts. Here we benchmark the Palabos software against the ANSYS commercial software. The Palabos environment does not offer the fastest LB implementation as it compromises raw speed with flexibility and reusability. Palabos achieves around two millions of site update per second (2 Msup/s) on a single core machine, for a D3Q19 simulation, whereas highly optimized LB implementations report around 6 Msup/s[20, 21]. However, Palabos scales very nicely on a large number of cores. Efficiency of the order of 80% have been observed on the CADMOS 16k cores IBM Blue Gene P machine.

The benchmark we propose here is a time-dependent flow in the synthetic aneurysms

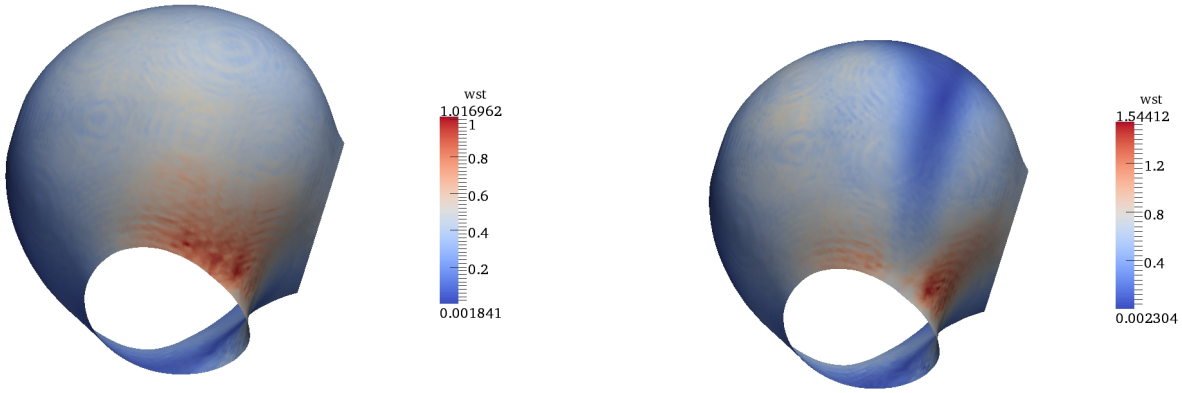

Figure 4: LB computations of the WSS with Palabos, with a Newtonian (left) and non-Newtonian (right) rheology. Note the difference in the scale for both panels. The parameter of the Carreau-Yasuda model are $\nu_0 = 5.6 \times 10^{-5}$, $\nu_\infty = 3.5 \times 10^{-6}$, $n = 0.357$ and $\lambda = 3.313$.

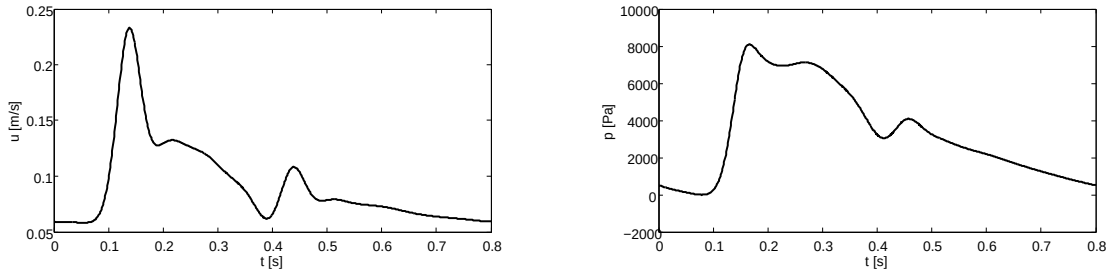

Figure 5: The inlet velocity (top) and outlet pressure (bottom).

described in section 3. The flow is imposed by a time dependent periodic ($T = 0.8s$) flat velocity profile at the inlet and two pressure profiles at outlets (see Fig. 5). These profiles were computed using the method developed by Reymond et. al. in [22]. The blood is assumed to be a Newtonian fluid, with kinematic viscosity $\nu = 3.283 \cdot 10^{-6}$ m$^2 \cdot$ s^{-1} and density $\rho = 1066$ kg $\cdot$ m^{-3}. The characteristic size of the geometry is taken to be the diameter of the inlet which is $L = 4.14 \cdot 10^{-3}$ m wide, and the length of the total geometry is of about 4 centimeters. Furthermore we took the characterisic velocity of the flow to be the systole peak velocity, $U = 0.238$ m $\cdot$ s^{-1}, which is reached at $t = 0.14$ s (see Fig. 5). Thus this leads to a Reynolds number of $\mathrm{Re} = UL/\nu = 293$.

The simulations are shown to have reached a stationary state after two time-periods. The ANSYS run contained 720273 elements whereas in the Palabos case there where 680080 nodes. The simulation took 75 minutes with the ANSYS solver on a four-cores

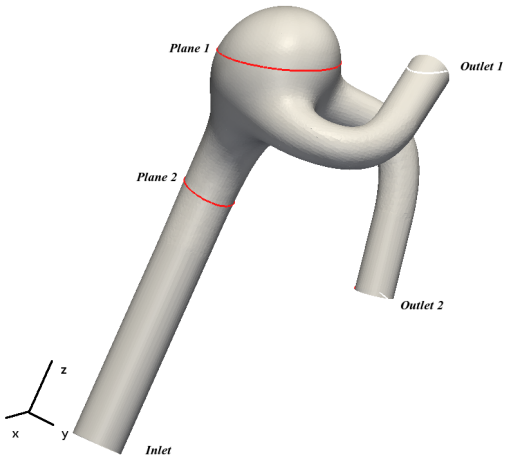

Figure 6: The geometry with the intersecting planes (represented by the red lines).

Xeon processor and 150 minutes with Palabos on eight cores of the same Xeon processors. The ANSYS solver is therefore shown to be about four times faster than Palabos. This greater cost for the lattice Boltzmann solver is essentially due to the fact that a very small time discretization is needed in order to solve stability issues. This problem could be at least partially solved by using grid refinment techniques. The simulation time can also be greatly reduced by using the Palabos solver with a larger amount of processors (because of the very good scalability of the lattice Boltzmann method, as mentioned earlier), which does not seem to be the case for the ANSYS solver.

In order to compare the accuracy of both solvers we compared the velocity fields on two planes (see Fig. 6 for the positioning of the comparison planes). As can be seen in Figs. 7 and 8, qualitatively the differences between both solvers is within a 10 percent range, and they are therefore in acceptable agreement[19]. These differences can be explained by the relatively low discretization of the space in these cases since the characteristic lengths of our system usually contain about ten grid points.

5 CONCLUSIONS

In this paper we discussed on-going research on the simulations of various processes in cerebral aneurysms, such as haemodynamics and thrombosis. Our developments are based on the open source Lattice Boltzmann Palabos software. More specifically we proposed a comparative benchmark between Palabos and the commercial finite volume solver ANSYS. In this early stage we showed a reasonable quantitative agreement between the results of both solvers. Although the ANSYS solver showed a better performance on a small number of processors, Palabos offers a free and publicly available framework which could be more efficient especially on larger parallel machines or GPUs.

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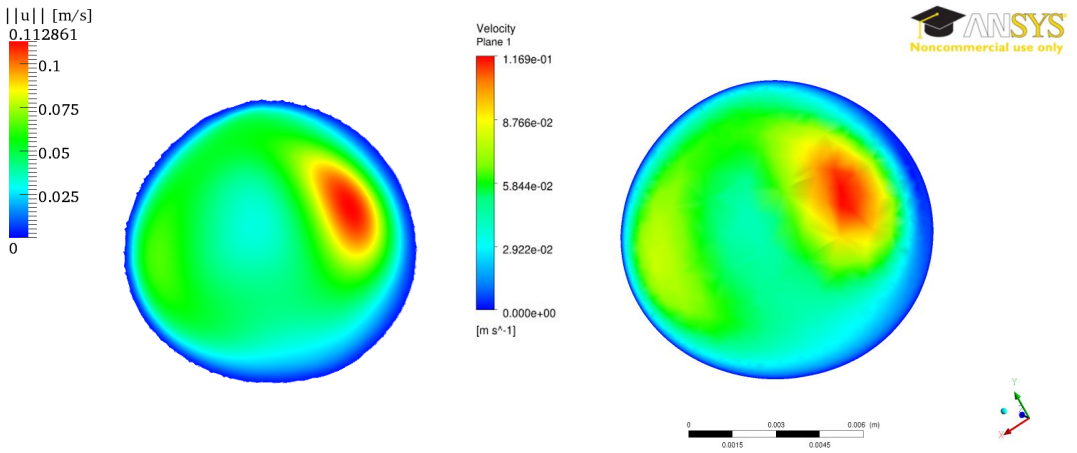

Figure 7: The velocity norm comparison between ANSYS (right) and Palabos (left) at plane 1.

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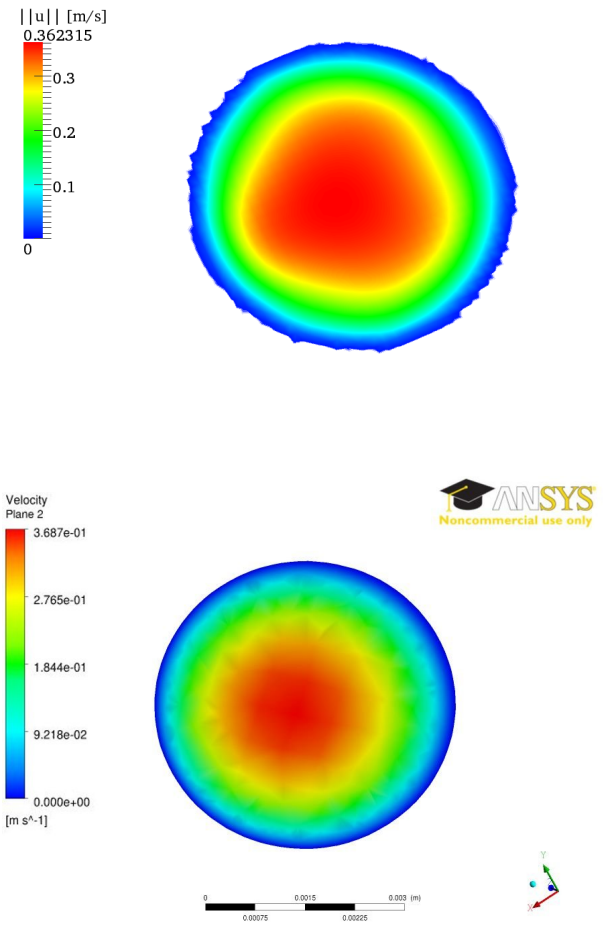

Figure 8: The velocity norm comparison between ANSYS (right) and Palabos (left) at plane 2.

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