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## An integrated environment for blood flow and heart simulation

nco<sup>1</sup>, Antonio Tadeu Gomes<sup>1</sup>, Daniele Lezzi<sup>2</sup>, Roger Rafanell<sup>2</sup>, Alfonso Santiago<sup>1</sup>, Mariano Vazquez<sup>1</sup> <sup>1</sup> Laboratorio Nacional de Computação Científica (www.lncc.br) - Brazil <sup>2</sup> Barcelona Supercomputing Center (www.bsc.es), Spain

www.eubrazilcloudconnect.eu | info@eubrazilcc.eu | eubrazilcloudconnect.eu/cloudscapebrazil2014

### A Pureblood simulator of the whole vascular system

Cardiovascular diseases have a huge impact on population, particularly people with a low- and middle-income. Since the early 1950s, there have been increasing efforts to develop computational models and simulationbased techniques in order to assess physiological and pathophysiological conditions accounting for the multiple time scales and levels of spatial organization present in the cardiovascular system (CVS). Applications such as diagnosis, treatment and surgical planning have been enormously benefitted from these complementary tools. Simulating a heartbeat is a complex, multi-scale problem. This means that many scales are coupled,

covering different orders of magnitude from descriptions of electrical propagation, cells arrangement into a spatial description, generally known as myofibre orientation; and up to the geometry of the cardiac chambers.

EUBrazilCC leverages the integration of heterogeneous supercomputing and virtualized infrastructures with the orchestration through the components integrated in the platform of two simulation codes from Brazil and Spain, addressing two complementary problems in cardiovascular modelling.

Alya Red: Computational heart

Alya Red is the in-house tool developed by CASE department in BSC, designed to model biomedical applications, specially optimized to run in HPC machines; in particular BSC supercomputer: Marenostrum.

This model solves the different equations involved in the phenomena separatedly: from the propagation of the electric impulse in the cardiac tissue, to the fluid dWynamics of the blood, including the deformation of the cardiac tissue and the Fluid-Structure interaction problem.

The latest medical imaging techniques provide high resolution geometries of the heart and provide information about the microscopic structure of the hart.

This geometries are meshed, and the different problems are solved using the power of Marenostrum supercomputer.



#### **One-Dimensional Arterial Blood Flow** Modeling

ADAN (Anatomically Detailed Arterial Network) is the model of the vascular system developed in the LNCC.

The mesh of the systemic arteries, result of years of research, includes over 2000 arterial vessels for an average man.

This geometry is processed by a solver which, by 1D finite elements, computes flow, pressure and lumen diameter of the vessels in each cardiac beat. There are two main advantages of this model over others. First of all ADAN features the most realistic vascular topology for a model in the scientific literature, and in second place it runs fast in regular  $computers thanks to the {\tt 1D} condensed formulation.$ 

#### Creating the most complex cardiovascular model

EUBrazil Cloud Connect will couple the Alya Red heart model with the ADAN model in order to deliver an unprecedented model of the blood flow circulation in the cardiovascular system, making possible to widen the range of cardiovascular scenarios that the model is able to address. In this sense, it is possible to study the effect of wave propagation back into the heart to analyze, for instance, the impact of aortic regurgitation on hypertrophy in the cardiac muscle, or the consequences of arterial stiffening into the heart efficiency. Likewise, changing parameters in the heart fu nctioning allows us to understand how this affects the pressure pulse conformation in detail. In any case, the coupled model naturally integrates phenomena taking place at such vascular entities (heart, systemic arteries). This use case will also demonstrate the coupling of heterogeneous infrastructures by leveraging on the available tools provided in the project to create and submit experiments.

The integrated environment for coupled simulations will allow for both parametric and full runs. Parametric runs, used for tuning the models, will be orchestrated by the COMPSs runtime in cloud environments. Full runs will use HPC resources at BSC and LNCC managed by COMPSs and the CSGrid middleware, and the coupling will be done through a connector

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in the cloud that regulates information flow between the two models over the network and across organization boundaries. The mc2 platform will provide a common user interface for these different types of runs.



From 2013 until earlier this year, Barcelona Supercomputing Center (BSC) formed part of EUBrazilCC, a project aimed at promoting cooperation between Europe and Brazil while supporting a scientific and knowledge-based society as the key to sustainable and equitable socioeconomic development. At the centre of this partnership were three use cases requiring cooperation between Brazil and Europe in the areas of data provision, services and expertise.

BSC's role was to provide support and development for the cardiology use case (Cardiovascular Simulation Services) and its subsequent implementation in two HPC systems. The goal of this use case is to analyse different working conditions of the cardiac muscle.

To this end, EUBrazilCC used the <u>Alya System</u>, BSC's simulation tool. Alya is fully developed in-house, from numerical methods all the way to parallel implementation, including mesh-generation and visualisation. The Alya Cardiac Computational Model (CCM) heart model was used in conjunction with the <u>ADAN model</u> (developed at <u>LNCC</u>) in order to provide an unprecedented model of blood flow in the cardiovascular system.

**Mariano Vázquez**, High Performance Computational Mechanics Group Manager at BSC, explains that "we are very excited about the potential that such a unique and complex model has for cardiovascular biomedical research. Once completely deployed and in production, hopefully before the end of the year, it will become not only the most comprehensive computational cardiovascular model in the world but also a great example of what research collaboration between Europe and Brazil can bring to the community."

The final results of the simulations are stored in the cloud database, ready to be retrieved by hospitals and laboratories as new data to be provided to the end-users, i.e. medical doctors.

The real breakthrough is EUBrazilCC's combination of these simulation tools under a cloud computing umbrella, including software coupling and access to both input and output data.

For EUBrazilCC the hope is that, in the relatively near future, doctors will use the results of this tool in the same way that they currently use imaging and radiology. A simulation will be run under specific conditions and these results will then be transferred to the doctor, rather as radiologists take X-rays before passing on the results. At the same time, the expectation is that medical researchers, depending on their expertise, will use these tools independently.

As part of the project, BSC also adapted the programming model <u>COMPSs</u> and the <u>PMES framework</u> to the necessities of several usage scenarios.

**Rosa M. Badia**, Workflows and Distributed Computing Group Manager at BSC, explains that "in EUBrazilCC we have demonstrated the features of the COMPSs programming model with real scientific use cases. Also, we have integrated the PMES/COMPSs framework on the project's open-source integrated platform, which features a whole software stack for the development and deployment of applications in distributed cloud federated infrastructures".

### **Strengthening the relations EU - Brazil**

The EUBrazilCC (614048) was a small or medium-scale focused research project (STREP) funded by the European Commission under the Cooperation Programme (FP7). BSC is also member of the consortium of other EU-Brazil projects, such as <u>HPC4E</u>, <u>EUBRA-BIGSEA</u> and <u>EuBrazilOpenBio</u>.

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### **Further information:**

dissemination@bsc.es - +34 93 401 58 37 (Núria Masdéu)

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