This welcoming winter in Barcelona Supercomputing Center Campus Nord hosted high performance computing-based simulations in engineering and environment with applications in bioengineering. Bioengineering has hugely vast scope incorporating principles of such sciences as biology, chemistry, mathematics, and computer science. And the seminar, that took place on 14-16 of February 2018 allowed to familiarize one with trends or even new branches of the study of biological systems. These can be approached from various angles, but only personal or professional interest should guidance you as to master one of immense number of branches substantial time and dedication will be needed.

The complexity can be seen on example of biomechanics. It is aimed at studying of healthy systems in order to resolve diseases. There are different levels in systems and each has its own solutions. It may be easy to solve certain level but coupling solutions may cause errors. Microscopic properties have to be modelled and studied in a process of search for solution, meaning scaling of various organizational levels is required. Imagine simulation of whole heart by simulating each molecule. This is a difficult task, as researchers of different organizational levels use different vocabulary, principles and so on, that creates difficulties in communication in process of global problem solving. Certainly, there are other difficulties. Cells move, grow, function, communicate having nonlinear, inelastic, multi-scale behavior.

Interconnectivity creates obstacle that may be concealed from beginning. And seminars like high performance computing-based simulations in engineering and environment provide valuable opportunity to discover and research topics of concern with support from industry and academic representatives, who also can become powerful connections. From supercomputer operation to data visualization, from stretching a blood cell to fluid mechanics in heart, all the advanced knowledge was shared by incredible speakers with years of experience and passion towards their job in three intense days. Such event can be a fantastic experience for curious, seeking for inspiration and development people.

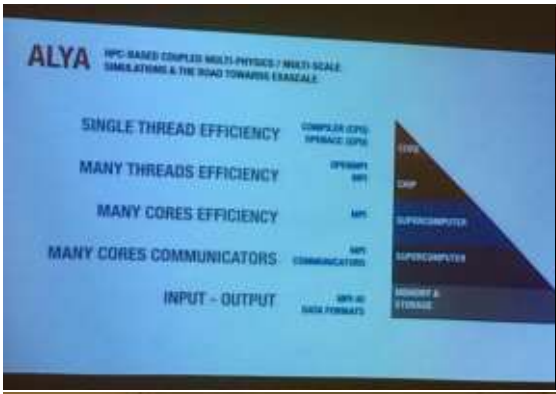
With the fast growth of computational performance and hardware scalability in recent years, High Performance Computing (HPC) have allow to perform from molecular dynamics to organ level simulation even more realistic physiological and multiphysics coupled simulations. PATC course has given a broad panorama in HPC based simulations of molecular and biological systems, computational chemistry, computer-aided design drugs (CADD), biomechanics, electrophysiology and hemodynamics. It combines, lectures from distinguished researches and hands on simulations using computational recourses that Barcelona Supercomputing Center offers with their supercomputer "Marenostrum".

Using HPC has a great impact on industrial applications like insilico trials for CADD, prosthetics development, as well as in clinical applications like risk fracture prediction and research application in different fields. Furthermore, this course gives an introduction to cloud HPC using Microsoft Azure, which helps to explore the dynamic scalability that they offer to fit each research application. Additionally, they offer the opportunity to build our own private HPC cluster and navigate through their interface.

This course also gives an approach of how tissue properties are acquired and translated to material properties for computational simulations. Using different methodologies like medical images obtained from CT scans or mechanical tests, tissue properties were acquired and mapped into 3D patients specific geometry model to simulate biomechanical behaviors. In addition, to validate simulations there are many approaches like plotting stress strain curves and comparing with tissue samples data.

A crash course on data visualization, show us that data visualization from simulations, is an important part for showing our research results. Data in numeric or text format can be quite confusing so data representation in a visual format helps to interpret results more quickly and easy, and highlights the important results.

I highly recommend this course as it gives a wide perspective and the latest trends of how HPC helps in actual industrial, clinical and research applications allowing to achieve more realistic multiphysics simulations. Furthermore, it gives a brief introduction to cloud HPC scalability and flexibility to adapt computational resources to the application requirements.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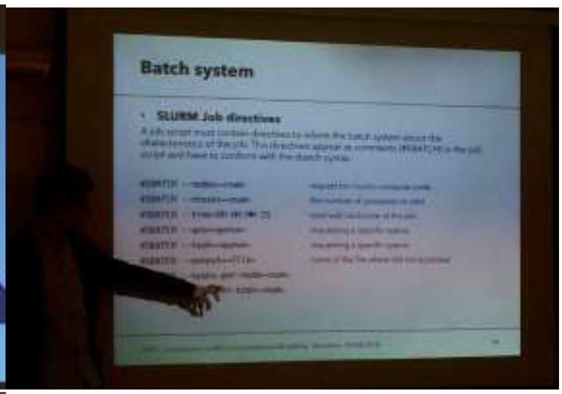
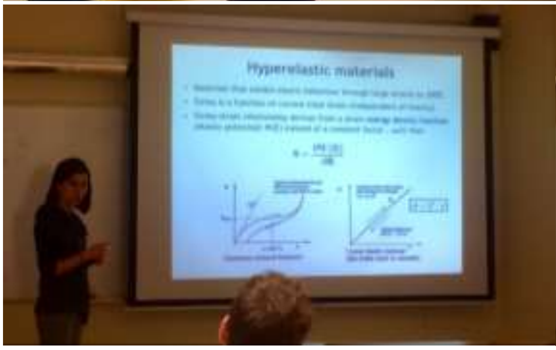

Batch system
SLURM Job directives


Bone anatomy
Cortical (compact) bone: typically 15-20GP in adults
Cancellous (spongy or trabecular) bone: 13-17GPa
Articular cartilage
Compact bone
Spongy bone


Hyperelastic materials


Computational Cardiology

In February 2018 the Partnership for Advanced Computing (PRACE) hosted a training event on HPC-based simulations, engineering and environment with applications in bioengineering at the Barcelona Supercomputing Center (BSC).

We started out Wednesday morning with introductory talks about computational mechanics for bioengineering applications and HPC in computational modeling. After lunch we were ready to dive more deeply into the matter: In the context of modeling blood flow on a cellular level, we learned about different strategies to increase performance and got our hands dirty running a simulation of the deformation of a single blood cell and another one modeling blood flowing trough a pipe on BSC's supercomputer MareNostrum 4. The last talk of the day was on parallel algorithms for computational mechanics and gave us a good overview on computer architecture, performance aspects as well as on parallelization paradigms.

The second day was all about different applications of HPC in biomedical engineering including a model of the human bone to predict osteoporotic fractures, in-silico guided drug discovery and HPC in metagenomics.

Day three started with a somewhat unexpected topic: Data visualization for researchers. Honestly, I had no idea what there is to know about the visual aspect of scientific communication before listening to graphic designer Guillermo Marin, who left me highly motivated to improve the visualizations in my future talks and posters. In the following talks we heard more about simulations for drug discovery, followed by talks about the Alya Red cardiac computational model and on fluid structure interaction in the cardiovascular system.

In the evening we went to the nearby church Chapel Torre Girona (photo), which is located at the banks of a small pond in a lovely little park at the Polytechnic University of Catalonia. Believe it or not, this nice and quiet spot is where MareNostrum is located.

Back home writing this report, I can say, that I got many new inputs and connected to many like-minded male and female colleagues. All told, I really enjoyed my time at BSC.

PATC Course: HPC-based simulations, Engineering and Environment with applications in Bioengineering

The course took place at the Barcelona Supercomputing Center (BSC), the leading supercomputing center in Spain. This gave the attendants an opportunity to have access to MareNostrum 4, which is the third most powerful supercomputer in Europe.

The three-day course offered an overview of what high performance computing (HPC) is and why it matters. The first day, lectures were about the basics behind HPC giving a panorama on computational tools and parallelization. Speakers presented Alya, the multi-physics and multi-scale code developed in the BSC to efficiently solve a wide range of computational problems. They also gave us an introduction about computational modelling from a multiscale point of view, showing applications from the molecular level to the organ level. The two last days, lectures were into a deeper explanation of specific research areas related to projects BSC are carrying on, such as molecular medicine, computer-aided drug design and biomechanics of the musculoskeletal and the cardiovascular system. In addition to the theoretical sessions, two hands-on sessions were carried out. Both sessions were very useful to put on practice the explained concepts and to solve real problems using MareNostrum 4 supercomputer.

Personally, the content of the course has given to me new and interesting resources which may help me to advance in my current and future studies. I'm a PhD student researching on the topic of computational modelling and simulation in the field of cardiac electrophysiology. Thus, lectures related with the biomechanics of the cardiovascular system specially aroused my interest. It was very exciting to be able to see what other researchers are doing in the same field and to find out the huge impact HPC-based simulations could have for healthcare improvement.

MareNostrum supercomputer at Barcelona Supercomputing Center

The three days workshop started on Februaruy 14th with an introduction on the general idea of HPC, the structure of supercomputers, etc. It was then followed by a course on the most frequently used Linux syntaxes in handling files (transferring, running, etc.) in an existing supercomputer which was quite practical and helpful. Different groups with different backgrounds presented the modeling and computational tools they had developed or used, and explained the necessity of HPC in solving problems they deal with. Dr. Zavodszky from University of Amsterdam presented 'HemoCell' which was basically a computational platform for calculating dynamics of blood flow and also deformation of blood cells. During the hands-on session, we found the opportunity to run a problem with 'HemoCell' on MareNostrum, the HPC facilities at Barcelona supercomputing center. Dr. Houzeaux presented the cons and pros of different existing paralleling algorithms. This session gave me an idea of which algorithm suits most for my own job at University of Liege. The workshop started the next day by a session on image-based finite element modeling of femoral bone to predict fracture risk. We also found the opportunity to segment a bone in ITK-Snap. Next Session presented by Mr. Podesta from Microsoft gave us an overview of the wide spreading concept of cloud computing, a new and relatively cheaper way to access supercomputing capabilities. Afternoon classes were on using computational molecular mechanics to design new drugs, based on the idea of receptors at the cells membrane switching different intra-cellular signaling pathways on/off. This session highlighted the importance of HPC in reducing costs and speeding up the process of designing new drugs. The last day started with a session on different ways of visualizing data to convey the message of a research as efficient and fast as possible. Next session was on application of molecular dynamics in drug discover which was more technical than the one was presented the previous day. The first session on the afternoon was on the theoretical basics of fluid-structure interaction and a couple of examples to show few phenomenon in nature where fluid-structure interaction plays an important role. The workshop ends with a session on introducing Alya Red, a computational platform to simulate heart performance which is in turn a complex and multi-physics problem requiring HPC techniques to solve numerically.