BOB Operation Report - FCT supercomputing cluster installed at MACC

October, 2020
EXECUTIVE SUMMARY

BOB is a supercomputing cluster donated by TACC to FCT and installed at MACC. It was inaugurated in July 2019, beginning at that time its pilot and testing phase.

During the period under review in this report, a restricted set of entities were invited to participate, to validate the basic set of computational services and to achieve operational stability.

In the absence of a dedicated operational team, this pilot phase was accomplished by the joint effort and dedication of collaborators from the following entities: FCT, UMinho, INESCTEC, LIP and INCD.

By the end of 2019, tune-ups and troubleshooting were carried out, especially with the storage sub system, a high-performance data storage system whose final configuration stabilized in December.
During the pilot it became evident the inability of Riba d'Ave data centre to ensure total cooling needs for BOB, as well as the unavailability of NOS to improve its facilities for this purpose. This represents a limitation of 35% in the computing capacity of BOB, persisting to the present time. There was also a refusal to respond to requests for quotations to upgrade the current 1 Gbps NOS connectivity, or to install low level transmission operator services.

With all the contingencies and difficulties of the pilot phase, and to avoid a negative user experience, the initial enrolment of new users was performed gradually and without widespread publicity.

This report shows that even with all the contingencies and difficulties encountered in this initial phase, the capacity used in BOB has had a sustained growth, having registered in September a utilization of more than 50% of the available capacity. During the pilot, over 32 million core-hours of processing time took place, involving more than 20 user entities from north to south of Portugal, covering various areas of knowledge. This is a result that is considered highly encouraging and validates the great usefulness of this type of resources, as well as the national capacity to use them.
Currently, due to an increase in the number of orders received, it was necessary to start implementing a quota policy to try to ensure fairer models of access to the computational resources.

The pilot will end with the evolution of BOB usage to more formal processes of access transparency and service security, which are being finalized through a set of administrative instruments, such as FCT’s regulation for access to computer resources and the operational support agreements, essential to frame the offered services.

FCT has already taken the first step in the next operational stage of BOB, by opening a public call for access to computer resources for the scientific community and is currently on the process of evaluating the proposals and deciding on computational resources attribution.

**CAPACITY USAGE**

The operational computational system contains 8,320 CPU cores, which corresponds to 6.1 million potential core.hours of processing capacity available each month, not considering the time for BOB maintenance. The total computational system made available by TACC would be capable of providing 9.3 million core.hours per month, free from the cooling limitations referred previously.
Definition of core.hour = processing hours multiplied by the number of processing units used in parallel. Term commonly used in Supercomputing as a unit for quantifying CPU usage. This general definition may have variants in the general definition if, instead of using generic CPU, specialized units are used, such as GPU.

Each microprocessor may have several CPU cores. For example, in each node of the BOB HPC cluster, there are two CPUs, each with 8 cores.

The following graph shows BOB's capacity utilization in September 2020:

Figure 1 – Bob usage profile
The following graphs show the monthly evolution of capacity utilization in core hours (Fig. 2) and the number of different users (Fig. 3) per month.

Figure 2- Monthly usage evolution, from July 2019 to September 2020.
Figure 3 - Monthly evolution of the number of distinct users, from July 2019 to September 2020. Each point represents the number of different usernames - by project or by institution - that used the machine in that month.

(*) In December 2019 the storage system upgrade took place which led to a general system shutdown.
The following graph shows the consumption of core.hours per user institution until September 2020.

![Bar chart showing core.hours per institution from July 2019 to September 2020. The highest consumption is by UMinho, followed by UCoimbra and ULisboa. Other notable institutions include LNEC, ITQB-NOVA, UAlgarve, ISEL, UAveiro, UNovaLisboa, LIP, MACC, INEGI, IPATIMUP, UPorto, INESC TEC, DTx COLAB, and UÉvora.]

*Figure 4* - Number of core.hours per institution from July 2019 to September 2020. Acronyms in detail in Table 1.
The following graph shows the consumption by region, according to the user institution.

Figure 5 - Percentage of core.hours by region NUT II from July 2019 to September 2020.

AML – Área Metropolitana de Lisboa.
The following graph shows consumption by scientific areas, from July 2019 to September 2020:

- **30%** for Mechanical Engineering and Engineering Systems
- **22%** for Physics
- **19%** for Materials Science and Engineering
- **11%** for Chemistry and Chemical Engineering
- **9%** for Neurosciences, Ageing and Degenerative Diseases
- **9%** for Civil and Mining Engineering
- **9%** for Biomedicine
- **7%** for Experimental Biology
- **4%** for Electrical Engineering and Computer Engineering
- **4%** for Environment and Global Changes
- **4%** for Biological Sciences
- **2%** for other/recent activity

*Figure 6 - Percentage of core.hours used by scientific area between July 2019 and September 2020*

Note: The information presented is based on user surveys conducted in March and April 2020. In the absence of a specific answer, the scientific area was estimated through the affiliation of the projects or users.
The following tables lists the requested computational projects.

**Table 1 - User institutions from July 2019 to September 2020:**

<table>
<thead>
<tr>
<th>Region NUT II</th>
<th>Institution</th>
<th>Subject</th>
<th>Scientific Areas</th>
</tr>
</thead>
<tbody>
<tr>
<td>NORTE</td>
<td>UMinho - Universidade do Minho</td>
<td>Polymers engineering</td>
<td>Materials Science and Engineering</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Mechanical Engineering and Engineering Systems</td>
</tr>
<tr>
<td></td>
<td>LIP - Laboratório de Instrumentação e Física Experimental de Partículas</td>
<td>Physics</td>
<td>Physics</td>
</tr>
<tr>
<td></td>
<td>INESCTEC - Instituto de Engenharia de Sistemas e Computadores, Tecnologia e Ciência</td>
<td>Genetics</td>
<td>Biological Sciences</td>
</tr>
<tr>
<td></td>
<td>DTx - Digital Transformation CoLAB</td>
<td>Several</td>
<td>Electrical Engineering and Computer Engineering</td>
</tr>
<tr>
<td></td>
<td>INEGI - Instituto de Ciência e Inovação em Engenharia Mecânica e Engenharia Industrial</td>
<td>Several</td>
<td>Mechanical Engineering and Engineering Systems</td>
</tr>
<tr>
<td>CENTRO</td>
<td>CICECO - Instituto de Materiais da Universidade de Aveiro</td>
<td>Materials science</td>
<td>Chemistry and Chemical Engineering</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Neuro inflammation; Drug discovery</td>
<td>Neurosciences, Ageing and Degenerative Diseases</td>
</tr>
<tr>
<td></td>
<td>UC - Universidade de Coimbra</td>
<td>Neuroscience and Cell Biology</td>
<td>Chemistry and Chemical Engineering</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Physics</td>
<td>Neurosciences, Ageing and Degenerative Diseases</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Physics</td>
<td>Physics</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Physics, Lattice</td>
<td>Physics</td>
</tr>
<tr>
<td>ÁREA METROPOLITANA DE LISBOA (AML)</td>
<td>UL - Universidade de Lisboa (Técnico)</td>
<td>Mechanical engineering</td>
<td>Mechanical Engineering and Engineering Systems</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>Plasmas and Nuclear Fusion</td>
<td>Physics</td>
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<tr>
<td></td>
<td></td>
<td>Particle Physics</td>
<td>Physics</td>
</tr>
<tr>
<td>UL - Universidade de Lisboa (FCUL)</td>
<td></td>
<td>Molecular Dynamics</td>
<td>Chemistry and Chemical Engineering</td>
</tr>
<tr>
<td>IDL - Instituto Dom Luiz</td>
<td></td>
<td>Climate change</td>
<td>Environment and Global Changes</td>
</tr>
<tr>
<td>ISEL - Instituto Superior de Engenharia de Lisboa</td>
<td>Machine Learning and Optimization Problems</td>
<td></td>
<td>Electrical Engineering and Computer Engineering</td>
</tr>
<tr>
<td>LNEC - Laboratório Nacional de Engenharia Civil</td>
<td>Hidraulics, Coastal modelling</td>
<td></td>
<td>Civil and Mining Engineering</td>
</tr>
<tr>
<td>FCT-UNL – Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa</td>
<td>Molecular chemistry</td>
<td></td>
<td>Chemistry and Chemical Engineering</td>
</tr>
<tr>
<td>ITQB-UNL - Instituto de Tecnologia Química e Biológica</td>
<td>Biotecnology</td>
<td></td>
<td>Biological Sciences</td>
</tr>
<tr>
<td>ISQ – Instituto de Soldadura e Qualidade</td>
<td>No information, Recent activity</td>
<td></td>
<td>Materials Science and Engineering</td>
</tr>
<tr>
<td>ALENTEJO</td>
<td>UE - Universidade de Évora</td>
<td>AstroPhysics</td>
<td>Physics; Maths</td>
</tr>
<tr>
<td>ALGARVE</td>
<td>UALG - Universidade do Algarve</td>
<td>Genetics</td>
<td>Biological Sciences</td>
</tr>
<tr>
<td>VÁRIAS REGIÕES</td>
<td>EDP</td>
<td>Energy</td>
<td>Electrical Engineering and Computer Engineering</td>
</tr>
<tr>
<td></td>
<td>Vestas</td>
<td>Energy</td>
<td>Electrical Engineering and Computer Engineering</td>
</tr>
</tbody>
</table>
After having finished the experimental operation cycle and BOB’s trials, it is important to perform a brief SWOT analysis of the entire system, in order to support management decisions, of something that is currently the biggest computational resource of RNCA – National Network of Advanced Computing.

**Strengths**
- General purpose CPUs
- High compatibility of Intel architecture with leading HPC software solutions
- High density interconnect
- Easy to setup
- Currently tested and in a growing phase of stable operation

**Weaknesses**
- Low energy efficiency
- Outdated accelerator processors
- High hardware failure rate
- Cooling limitations imposed by the data centre, namely in the interconnect
- Power supply limitations imposed by the data centre
- Inadequacy to perform some AI applications in high demand

**Opportunities**
- Increase the number of computational services
- Use as a learning platform for developing supercomputer operation capability as well as for new users
- Reinforce the computational capacity made available to competence centers
- Use as a platform for testing different computing environments

**Threats**
- High level of obsolescence
- Outdated architecture (Single CPU) can significantly limit the application domain in the future
- Substantial increase in operating costs, namely due to hardware breakdown
THANK YOU