Technology Transfer in Computing Systems

D3.30: Individual TTP30 abstract

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TETRACOM D3.30: Advanced Computational Drug Discovery Technologies using High Performance Computing Architectures (ACDDT-HPC)

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The development of new drugs is a long and costly process. This process usually starts in a laboratory, where a large number of chemical compounds is tested for effectivity against specific factors involved in the targeted disease. These experimental tests imply high costs (equipment, chemical compounds, waste management, etc) and long development times. Computational Drug Discovery aims to reduce these costs by making predictions on the effectivity of the compounds, so that the number of tests can be effectively and drastically reduced. The expected impact of this project is to exploit Drug Discovery methodologies, previously developed by the Bioinformatics and High Performance Computing (BIO-HPC) research group, and to provide services based on these technologies to pharma/biotech companies working on the Drug Discovery field at the national (Spain) and international (EU) levels, through the expertise and background of the partner company, Artificial Intelligence Talentum SL (AI Talentum).

The technology that will be transferred is already in a very advanced state (TRL: 7) and has already been tested in an academic environment (several scientific papers, based on results achieved with technology, have already been published; see http://bio-hpc.eu/publications/). Therefore, during this TTP we will focus only in the following tasks:

- Porting the technology to the cloud, and upscale it to be ready for mass usage.
- Preparation of marketing materials to promote the services derived from the technology.
- Commercialization of services based on the technology.
- Development of the contract signed Drug Discovery projects.

AI Talentum is a novel company with an important scientific, technological and marketing profile, that has specialized in delivering Artificial Intelligence solutions based on Big Data modeling. Most of its staff are PhDs in areas like Chemistry, Physics, Mathematics and Computer Science, and it is therefore an ideal partner for this project. The company will mainly benefit from the economic aspects for the project, which will give rise to a new line of services. At the same time, the research group at UCAM will benefit from the extended visibility for their technology. This extended visibility is expected to yield new scientific collaborations, which will result in new publications and funding applications, as well as feedback, which will help to improve the technology.

The technology of this TTP consists in a software package which bundles together some well-established tools used in bioinformatics, related to docking small chemical molecules on protein receptors, with some other tools developed at the BIO-HPC group. When put together, and installed on a HPC cluster, this software package allows an operator to quickly deploy a series of computational tasks to solve different challenges related to the discovery of new drug leads or the optimization of already known active compounds. These computational tasks are effectively distributed to the different machines in the HPC cluster in order to produce a set of semi-processed results in a quick and cost efficient way. These results can later be retrieved by the operator, and studied to extract conclusions from the calculations and prepare a report.

During the TTP, and once the technology had successfully been ported to work on cloud computing infrastructures, it was tested again on three commercial projects: a molecular mechanistic study project for the University of Iceland, a compound optimization project for the University of Hong Kong and a peptide docking project for the University of Naples Federico II. The details for the projects are subject to confidentiality, but besides complete customer satisfaction, the compound optimization project also achieved to identify a potential lead for a new drug, as one of the suggested compounds was found to exhibit nanomolar activity.