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Exploitation of Massively Parallel Architectures for Drug Discovery

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The discovery of new drugs can be accelerated thanks to Virtual Screening methods (VS), which predict potential active compounds using computer simulations. Unfortunately, the accuracy of their predictions is restrained to a lack of enough computational resources for scientists. Classically, scientists have programmed their VS codes in supercomputers, but these infrastructures are usually expensive and not all research groups can access them. In the last years, a new alternative computational architecture has emerged, named Graphics Processing Units (GPUs), which provides a performance similar to a supercomputer but for a smaller fraction of their price.

In the last five years, many scientists and programmers have spent lots of time learning to program these new devices and testing how to adapt old legacy codes or designing new ones from scratch, with different levels of success. In the first years, GPU technology was still immature and there was a lack of efficient tools for its new programming paradigm, so although it was a promising technology, its practical applicability was not clear at all since there was not a standard approach for its exploitation. But later, support from one of the main GPU manufacturers (NVIDIA) and their CUDA language "one ring to rule them all", changed completely the landscape, and now it takes much less time to learn how to program a GPU, and its computational power is growing constantly.

Only disadvantages that should be mentioned are the minimum computer science background required for its application, which can exceed the classical sequential programming knowledge of scientists of the PC-era, but which should not prevent nor fear them for learning it.

So it is clear that for computationally intensive VS methods, such as docking, Molecular Dynamics, and the like, GPUs have evolved as a mature alternative to supercomputers, and even more, a cheaper and much less power consumption one.

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