

Accelerating Molecular Modeling with oneAPI and Intel® FPGA Accelerators

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The Institute for Advanced Chemistry of Catalonia (CSIC) focuses on developing new techniques to improve the field of molecular structures. The challenge with iterative methodology for verifying the structure of molecules is that it requires computational effort in the verification phase. The scientists at CSIC turned to the Barcelona Supercomputing Center (BSC) and their High-Performance Computing team for help. The HPC team at BSC determined that an FPGA would be the best fit for the CSIC algorithm. Developing any acceleration card takes time and effort. To solve this development challenge, BSC turned to Intel Titanium partner BittWare, part of Molex. BSC could solve their development problem by buying an off-the-shelf BittWare IA-840f card, which uses an Intel Agilex® 7 A027 device. The results of using Intel® oneAPI Base Toolkit (Base Kit) and the BittWare IA-840f acceleration card surpassed expectations. The algorithm executed in 61 seconds on the new platform and 41 seconds for the customized accumulator version, which is a 233x improvement over the CPU and about 13x improvement over the initial OpenCL Intel® PAC with Intel® Arria® 10 GX FPGA solution.¹

Industry
Research

Organization Size
10,001+

Country
Spain

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¹ For more complete information about performance and benchmark results, visit <https://www.intel.com/content/www/us/en/customer-spotlight/stories/bsc-bittware-customer-story.html>