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# Interdisciplinary Computational Projects Utilizing the HPC Cluster

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## **Interdisciplinary Computational Projects Utilizing the HPC Cluster**

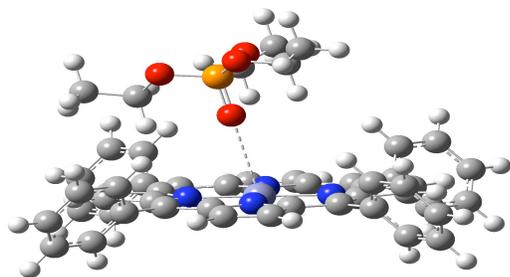
*Final Report for Thinkfinity Grant  
Cornerstone 3*

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The Harold Blancke Professor of Physical Chemistry

We received funds from the Thinkfinity Project towards the acquisition of scientific computational software, which would become available to all users in the academic community (both faculty and students) and would be deployed in the High Performance Computing Cluster (HPCC) and as well as in local workstations. In particular we purchased unlimited licenses for LINUX and Mac OSX platforms of the GAUSSSIAN09 package, along with unlimited licenses for its graphical interface companion GaussView 5.1 for Windows and Mac OSX systems.

Since we experienced some unexpected delays related to changes in the ITS division and to the approval of the License agreement for some of this software from the Legal Department of the University, the deployment of the entire project was completed just last week, making it impossible for us to submit intermediate progress reports.

The computational component was successfully installed on the HPCC and on some local Linux workstations. We performed *ab initio* Molecular Modeling calculations at very fast rates, approximately 10 to 20 times faster than the average of previously performed computations. Several research projects have been completed. Among them are some Internal Coordinate calculations, studying the pathways of important physical absorption interactions that take place in Gas Chromatography used in Forensic Chemistry.



Two distinct molecular groups were allowed to approach each other from various angles and the energy of their interaction was measured. The analysis of the outcome showed which atoms of these molecules interacted (displayed above, connected with the dashed line) and what was the strength of their binding. This information allowed us to optimize the settings of the experimental procedure used for the separation and identification of the involved molecules.

This project has already affected both the students and faculty of Science at Pace University. The graphical interface program has been installed on computers that are easily accessed by the students. At these locations the users prepare the input files and they submit the computational jobs to either local workstations or to the HPCC. After the completion of their runs they download the output files and analyze the results.

This procedure proves to be an exceptional teaching tool for research and will become a part of the curriculum for the foreseeable future.

This project has the potential to change the future of teaching the molecular structure of matter. In the upcoming weeks, communication protocols between end-users and computing stations will be completed in its entirety and optimized. Both the chemistry and biology educational curricula will be linked together and new training modules will be developed.

Due to the aforementioned delays, we have started (in association with the new cluster administrator) the installation of related classical dynamics packages on the cluster. Simulation cells of the topoisomerase IA carboxyl-terminal domain have been prepared and tested on smaller computational engines. These simulations will be directly compared to comparable simulations on the HPCC cluster. Initial simulations testing the speed and scale-up of the cluster will be performed; however, usable data will immediately become available for analysis.