Optimizing a Biophysics Supercomputer Application

Kim, Haram

The primary objective of this investigation is to improve the efficiency of the UltraScan-III software, which uses supercomputer environments to study soluble molecules in analytical ultracentrifugation (AUC) experiments. To accomplish this, a novel solute grid generation method was developed based on the Faxen solution of the Lamm equation (which describes the behavior of solutes under ultracentrifugation), in order to avoid redundant calculations in the software's grid-based algorithms. It was hypothesized that the overall number of calculations required for an analysis would be reduced, without loss in accuracy, by using the Faxen-derived grid mechanism. The Faxen-derived method was then compared against both a theoretically perfect but computationally expensive numerical grid and the currently implemented regularly spaced grid using a computer program developed by the researcher, and found to be a significant improvement over the regular grid. This result confirmed the hypothesis that efficiency could be improved through the use of a Faxen-derived grid and demonstrated the Faxen mechanism's suitability for use in the UltraScan software.

Awards Won: