**Automated Web- and Grid-Based Protein Phasing with *BnP***

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*BnP* is a protein structure-determination package that couples the direct-methods program *SnB*, used to locate heavy-atom substructures, with parts of the protein-phasing suite *PHASES* [1]. Thus, *BnP* provides an automated pathway from intensity data to an unambiguous protein electron-density map. In large or difficult cases, substructure determination can be a bottleneck. However, the *Shake-and-Bake* algorithm that is used to phase substructures can be readily adapted to a parallel computing environment and throughput increased in direct proportion to the number of available nodes.

Versions of *BnP* with a Java interface are currently available from http://www.hwi.buffalo.edu/BnP/. In addition, a new interface has been developed in PHP, a general-purpose scripting language that is especially suited for web development and allows users to run *BnP* from a browser displaying dynamically created web pages. It supports remote computation and has the capability of distributing multiple parallel jobs over a computational grid. The PHP version has been implemented on a stable prototype grid that was developed at SUNY Buffalo's Center for Computational Research and includes hardware at several different locations. An elegant backfill facility provides access to idle CPU time on many machines and makes it available for *BnP* calculations without disturbing other jobs. This work was supported by NIH grant EB002057 & NSF ACI-0204918.

[1] Weeks C. M., *et. al*., *Z. Kristallogr*., 2002, **217**, 686-693.

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