

## W0624

**Adapting *BnP* for Different Computing Environments.** C.M. Weeks<sup>a</sup>, S.A. Potter<sup>a</sup>, N. Shah<sup>a</sup>, H. Xu<sup>a</sup>, M.L. Green<sup>b</sup>, R. Miller<sup>b</sup>, L. Pasupulati<sup>c</sup>, W. Furey<sup>c</sup>, <sup>a</sup>Hauptman-Woodward Inst., Buffalo, NY, <sup>b</sup>Center for Comp. Res., SUNY at Buffalo. <sup>c</sup>VA Med. Center, Pittsburgh PA & Dept. Pharmacol., U. Pittsburgh.

*BnP* is a protein-phasing package that provides a convenient pathway from intensity data to an interpretable electron-density map [1]. This pathway includes substructure determination using the powerful statistical minimal function, heavy-atom refinement, protein phasing, density modification, and skeletonization. Scripts can be created and executed automatically for chain tracing, graphical visualization, and refinement by external downstream programs.

*BnP* was first developed with a graphical user interface (GUI) that is written in Java and is suitable for both manual and semi-automatic operation. Recently, an option has been added that allows startup from a command line, thereby permitting a higher degree of automation and bypassing the GUI altogether. In addition, a new interface has been developed in PHP. This interface allows users to run *BnP* from a web browser, supports remote computation, and has the capability of distributing multiple parallel jobs over a computational grid. *BnP* is available at <http://www.hwi.buffalo.edu/BnP/>. This work was supported by NIH grant EB002057 & NSF ACI-0204918.

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