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BnP on the Grid. R. Miller^{1,2}, M.L. Green¹ & C.M. Weeks², ¹Center for Comp. Res. & Dept. of Comp. Sci., SUNY-Buffalo, ²Hauptman-Woodward Inst., Buffalo NY.

The Advanced Computational Data Center Grid (ACDC-Grid) consists of an integrated computational and data storage systems distributed throughout Western New York. A heterogeneous set of machines incorporated into this grid from the Center for Computational Research (www.ccr.buffalo.edu) include a 4000-processor Dell PentiumIII/Xeon cluster, a 64-processor SGI Origin 3800, a 78-processor IBM SP2, a 150-processor SGI-Intel PentiumIII cluster, an 80-processor Sun Ultra5 cluster, a 16-processor IBM340 cluster, a 604-processor Dell Pentium4 cluster, and a variety of IBM and SGI workstations. In addition, the ACDC-Grid includes Condor flocks in UB/CSE, the Hauptman-Woodward Inst., and the UB Dental School.

The ACDC-Grid was implemented to support the use of the protein-phasing package *BnP*. The *SnB*-based substructure determination portion of *BnP* is readily adapted to a distributed computing environment. The grid portal assembles the required *SnB* files and job management facility automatically determines the appropriate number of processors for each available compute system. The ACDC-Grid backfill service has automatically provided grid users with the ability to submit 4200 jobs and consume 500,000 CPU hours in a 6-month period without impact on other users. Research supported by NSF grant ACI-0204918 & NIH EB002057.