

2014 HPC User Site Census: Applications

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EXECUTIVE SUMMARY

This report is part of our HPC User Site Census series and provides an examination of the primary application software found at a sample of HPC user sites. We surveyed a broad range of users about their current computer system installations, storage systems, networks, middleware, and applications software supporting these computer installations.

Our goal in this analysis of applications is to examine the suppliers, products, and primary usage of the application software packages in use at all HPC sites. Using our primary usage categories, we have created two super segments: High Performance Technical Computing (HPTC) applications and High Performance Business Computing (HPBC) applications. We examine these two super segments in this report.

Key findings of the Site Census surveys include the following:

- 432 unique supplier-packages representing 867 mentions were listed by all sites: 665 were HPTC applications and 202 were HPBC applications. About three-fourths of HPTC packages and nine-tenths of HPBC packages are mentioned only once in the survey, indicating the diversity of application needs and the experimental nature of the HPC market.
- Chemical research, business intelligence, biosciences, fluid dynamics, and weather/environmental modeling were the top five HPC usage categories for application software. Weather/environmental modeling replaced structural analysis as the fifth-place usage category. Business Intelligence was the only HPBC usage category in the top five.
- The leading application software packages in HPTC were GROMACs, Gaussian, NCAR's WRF, ANSYS's Fluent, University of Vienna's VASP, and OpenFOAM. The leading application software packages in HPBC were Hadoop and those provided by Oracle and Amazon. All of these top packages were used at multiple sites.
- Of the top 11 HPTC applications (two tied for 10th place) by number of mentions, five were chemical research, two were fluid dynamics analysis, two were structural analysis, one was weather/environmental modeling, and one was biosciences. Of the top HPBC applications by number of mentions, six were business intelligence and four were MapReduce-based applications.
- Open source was the leading source of programs, with 38% of mentions. About 90% of the open source codes were reported by academic and government sites. Software developed in-house accounted for 31% of mentions, with commercial ISV packages accounting for 25%. Public software was represented with just 6% of mentions.

System vendors should work to support applications through a multi-stage process, which includes: basic programming support, development of applications support staff, porting of major codes, and development of vertical market expertise.