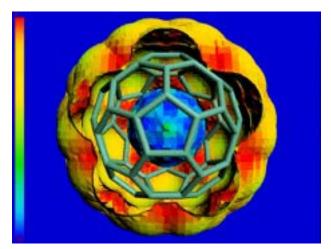


High Performance Solutions: VAMP on AlphaServers from Compaq

Leading edge computing for competitive research needs

Discovering and developing new products is a long and complex process. VAMP enables scientists to model greater numbers of molecules than ever before, improving their chances of product discovery. By running on Digital AlphaServers from Compaq, they can conduct more computations faster than ever before. Plus the impressive price/performance of AlphaServers helps to reduce overall systems management costs. Pharmaceutical, chemical, and biotech companies use VAMP on AlphaServers to reduce time-to-market of new products, decrease R&D costs, and ultimately gain greater profits.



Charge Density plot for Buckminster Fullerene This image of charge density surrounding a C_{60} molecule was created by VAMP. Image courtesy of Oxford Molecular PLC

VAMP Highlights

VAMP allows scientists to find new leads faster. With the advent of combinatorial chemistry came the ability to quickly synthesize thousands of compounds in a short period of time. VAMP is a powerful screening tool that enables scientists to find the few good candidates from the thousands or millions of compounds in their databases in order to develop innovative new products. In effect, it gives scientists the ability to find "a needle in a haystack."

The Compaq advantage

In the fiercely competitive world of product discovery, compute performance is critical. Products such as VAMP require enormous horsepower to work effectively. They greatly benefit from multiprocessor machines because of parallel processing capabilities. Alpha systems provide the best performance for customers' most challenging modeling needs. And Compaq protects its customers' investments with a clear upgrade path to even greater increases in performance



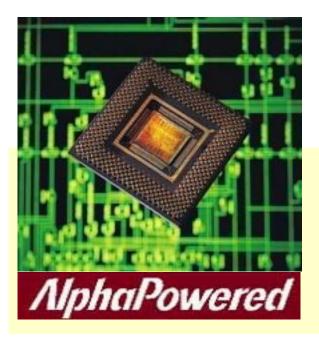
VAMP Highlights (continued)

VAMP is an extremely fast, accurate, and reliable semiempirical molecular orbital package that enables scientists to predict the likely structure and activity of molecules. Its top of the line electrostatics performance and its ability to integrate easily with popular chemical computing applications makes VAMP an excellent choice for rapid computational screening.

Developed by a research group at the University of Erlangen, Germany, VAMP uses quantum mechanical techniques to predict molecular electrostatics for developing more accurate QSAR, which helps scientists to estimate the shape of a molecule. With this information, scientists can begin to understand the effects of the molecule and determine if it will interact effectively with the target. VAMP is extremely fast, especially on large, parallel computers.

VAMP supports these methods:

- AM1
- MINDO/3
- MNDO
- MNDO/C and
- PM3



The Compaq advantage (continued)

Key Strengths

- Multiprocessor systems for high throughput as well as parallel and distributed computing
- The fastest microprocessor in the industry for unmatched application performance
- Reliability and robustness of Alpha systems and clusters of systems to easily support a large population of users
- Very Large Memory (VLM) for high-speed data searching and screening, enabling researchers to handle high volumes of data
- Integration support including custom integration services available to provide pre-tested, high performance configurations to meet each customer's specific needs
- Leading GIGAswitch and MultiSwitch 900 network backbones for the ultimate throughput in high performance networked computing
- Availability of a wide variety of computational chemistry applications on Alpha platform
- Ability to handle heavy workload without significant degradation of performance
- Excellent visualization tools to give users a better understanding of computational results, enabling them to make better business decisions

Find the compounds you want. Reduce time-to-discovery. Maintain your competitive edge.

Think Compaq and VAMP.

For more information, see <u>www.digital.com/onlinelab</u> or <u>http://www.ccc.uni-erlangen.de/</u> <u>clark/topics/vamp/</u>

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