ACCELRYS MATERIALS STUDIO DMOL³ ON HP PROLIANT SERVERS

Revolutionary modeling solution accelerates the rate of discovery

Solution brief
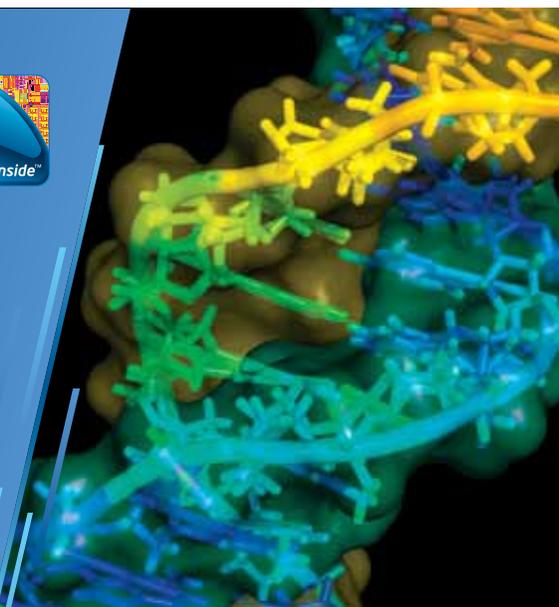
Processes speeding up

Whether you're a chemical researcher trying to identify a more effective medicine, or a manufacturer trying to determine a more efficient synthesis pathway, you rely on modeling at every stage of discovery. But as the rate of business accelerates, so must the rate of discovery.

Today, you need a modeling solution that can help you do more in less time for less cost. And HP and Accelrys can help by delivering Accelrys Materials Studio DMol³ running on HP ProLiant servers.

Unique approach to quantum mechanics

Helping you meet any research challenge with confidence, DMol³ is a density function theory (DFT) program with a long track record of successful commercial applications. With its unique approach to solving quantum mechanical equations, DMol³ has long been one of the fastest methods available for performing calculations—an advantage that becomes readily apparent in larger systems. With the addition of the B3LYP method, DMol³ achieves improved accuracy at accessible speed.

DMol³ is equally well-suited for performing a conformational analysis of a small molecule as it is for modeling catalysis on a metal surface. DMol³ has been applied to such diverse research problems as catalysis, semiconductors, reactivity combustion and more.

Example applications include:

- Study of the process of chemical vapor deposition

- Understanding the action of automotive catalysts
- Explaining the mechanism of polymerization reactions
- Investigating combustion techniques under extreme conditions

Faster methods, better results

Accelrys Materials Studio DMol³ running on HP ProLiant servers provides one of the fastest methods available for performing calculations—a very important advantage for larger systems. And new with this version of DMol³ with B3LYP, which requires significant memory, you can take advantage of the extremes of scale-out or scale-up offered by the HP ProLiant family, ranging from the scale-out HP ProLiant SL390s G7 servers to the massively resource-dense scale-up HP ProLiant DL980 G7 servers.

With its ability to model both molecular and solid state problems, the HP and Accelrys solution enables you to study the broadest possible range of problems in a single package. You can use DMol³ and HP ProLiant servers for:

- Modeling ligand binding during pharmaceutical discovery
- Understanding potential degradation pathways for drug molecules
- Designing new metallocene catalysts for polymerization
- Understanding the mechanism of supported metal catalysts
- Predicting band gaps
- Designing new solid state materials
- And much more

Your solution benefits

For computing centers, pharmaceutical development companies, contract research organizations and chemistry departments within higher education facilities, this HP and Accelrys solution offers impressive benefits:

- Increase computational screening rate by 50%
- Increase accuracy, reducing the number of false positives
- Model higher molecular weight ligands than with other methods
- Boost calculation performance using the in-core scale-up method on a HP DL980 Server with 1 TB or more of memory, or using the disk-based scale-out method with a cluster of 2-socket systems with 4–8 GB of memory per core

HP and Accelrys advantage

- **Fully integrated**: The solution is standards-based so it easily integrates with your existing infrastructure.
- **Fast time to user adoption**: The user-friendly interface complies with Microsoft® Windows® standards.
- **Comprehensive**: This solution includes a wide range of model-building and visualization tools.
- **Flexible client-server architecture**: You can run calculations on servers located anywhere on your network.

More speed, no compromises

DMol^3's emphasis is on speed—without compromising quantum mechanical accuracy. An efficient geometry optimization algorithm lets you predict minimum energy structures rapidly.

A transition state search employing a combination of LST/QST algorithms facilitates the evaluation of energy barriers. Using parallel versions of the DMol^3 code, you can tackle large problems and find the answers you need.

Member of the Materials Studio suite

DMol^3 is a component of the Accelrys Materials Studio software suite, and is accessed from Materials Visualizer, a common user-friendly interface that complies with Microsoft Windows standards.

Materials Visualizer offers a wide range of model building and visualization tools that allows you to rapidly construct models of systems, easily select DMol^3's and then run advanced quantum mechanics calculations.

The familiar user interface, together with Accelrys' training programs and the other components in the Materials Studio suite, ensures that even new users can use DMol^3 with confidence.

HP ProLiant DL980 servers – delivering confidence and reliability

Powered by the latest Intel® Xeon® processor technology, the HP ProLiant DL980 platform is a massively resource-dense scale-up server. Built on industry standards, the DL980 is designed to break through the boundaries of scale-out computing with the ability to handle the largest and most challenging applications and workloads.

With the goal of fast, easy deployments that you can customize and grow on demand, HP ProLiant DL980 servers maximize performance and efficiency. HP ProLiant DL980 servers:

- Reduce bottlenecks
- Improve throughput
- Boost performance
- Enhanced reliability
- Provide expandable memory
- Reduce your infrastructure costs

HP ProLiant SL390s servers – extreme scale-out solution

Powered by the Intel Xeon 5500/5600 series processors, the HP ProLiant SL390s G7 Server is part of the HP ProLiant SL6500 Scalable System family. Optimized for scale-out customers, the HP ProLiant SL390s G7 Server is designed to greatly reduce costs, maximize power efficiency and maintain total flexibility by sharing resources, power supplies and fans.

Delivered on an HP Cluster Platform, HP can configure, build, test and deliver complete cluster environments quickly, with maximum quality and reliability.

Bringing it all together

IT for materials science is not just about computation; it requires a complete IT strategy that encompasses computation, data management and more.

HP is uniquely capable of enabling a total IT solution for the sciences through the HP Converged Infrastructure model. Converged Infrastructure leverages HP's broad product set by bringing together servers, storage, network, management software and data center solutions into a single product and services offering that creates a complete environment for science and engineering.

In addition to HP ProLiant servers, you can also choose from:

- **HP X9000 Network Storage Systems**: Offering the ability to scale-out beyond traditional NAS in both capacity and performance. Designed to be extremely scalable, flexible and cost-efficient, the HP X9000 systems deliver excellent performance and a modular storage infrastructure to accommodate unprecedented storage growth and performance.
- **HP Cluster Management Utility**: Enabling cluster provisioning, management and monitoring, supported by HP across multiple Linux distributions.
- **HP Networking**: A key enabling technology in HPC clustering and other data center scale-up and scale-out solutions.
- **HP rack and power solutions**: Enabling deployment in existing facilities by offering maximum density and power efficiency.

Your next steps

Contact your HP and Accelrys representatives today and arrange for an assessment of your IT environment. Discover how Accelrys Materials Studio DMol^3 running on HP ProLiant scale-up or scale-out servers can create a revolutionary modeling platform that accelerates your rate of discovery.

For more information, please visit:

- www.hp.com/go/proliant
- www.hp.com/go/scale-up
- http://accelrys.com/products/datasheets/dmol3.pdf
- www.intel.com/products/processor/xeon/index.htm

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