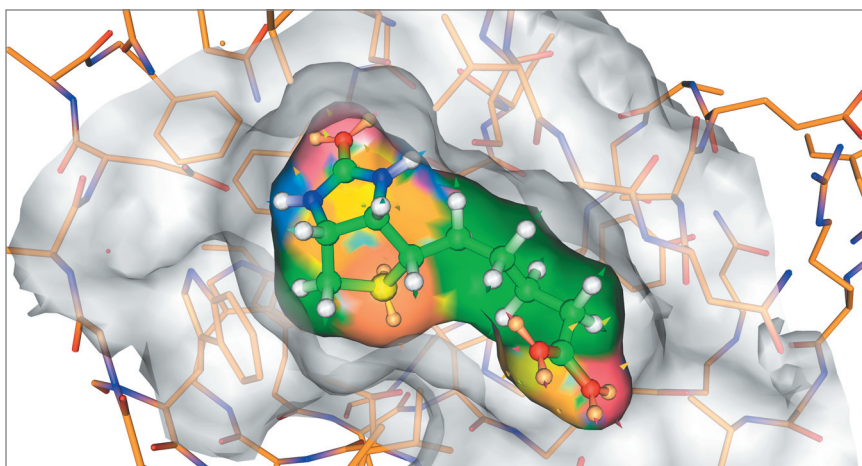


Molecular modeling utilizing the IBM BladeCenter QS21



Highlights

- ***Delivers a dramatic improvement in processing time for complex computational chemistry algorithms***
- ***Cell Broadband Engine multi-core technology helps speed mathematically intensive tasks***

A computational crisis

Computational chemistry is crucial for developing new drugs and materials, assisting the chemist in understanding data or sparking the challenge to find entirely new chemical objects. In particular, flexible ligand docking helps chemists identify molecules, or ligands, that interact with—or dock—to a receptor associated with a disease, and can often lead to potential cures. However, the processing power necessary for such computations presents challenges.

The solution to these challenges is SimBioSys® eHiTS® flexible ligand docking software running on the IBM® BladeCenter® QS21. The QS21 incorporates two Cell Broadband Engine™ (Cell/B.E.™) processors into a standard blade form factor. The Cell/B.E. processor is an asymmetric multi-core processor that is optimized for parallel processing and streaming applications. Unlike symmetric multi-core, cache-based architectures, which might not be able to handle streaming applications efficiently, the Cell/B.E. processor is designed to offer very high performance and fast response.

A 74x improvement in calculation time

eHiTS on Cell B./E. architecture dramatically speeds calculation execution times. In fact, the Lennard Jones 6-12 potential calculation ran 74x faster on an IBM QS21 BladeServer compared to a Dual-Core Intel® Xeon® processor-based server running at 2.4 GHz.



SimBioSys (www.simbiosys.com) ported eHiTS to Cell/B.E. architecture using the IBM Software Development Kit (SDK) for Multicore Acceleration Version 3.0. The SDK provides the libraries, tools and resources that businesses need to develop and tune applications for Cell/B.E. technology, and supports both Red Hat Enterprise Linux® 5.1 and Fedora 7.

Table 1 shows performance improvements achieved for additional eHiTs calculations on Cell/B.E. architecture compared to traditional CPUs at equivalent clock speeds. These are preliminary numbers, and as the code is not yet fully tuned or optimized, the final results are expected to be even more significant.

Table 1

Function ported and tested	Calculation speed improvement
Interaction energy calculation (H-bonds etc.)	34x
Steric clash determination	93x
Complete Flexible Docking with eHiTS	36x

Solving tomorrow’s problems today

The need for computational power is only going to increase. Researchers seeking to unravel the mystery of disease, and discover new drugs and materials must look to solutions that help them meet their need for increasing computational power. SimBioSys eHiTS running on BladeCenter QS21 can deliver the power organizations need to accelerate key algorithms and speed solutions to tomorrow’s problems today.

For more information

To learn more about this and other IBM solutions call 1 877 IBM-ACCESS (1 877 426-2223) to speak to an IBM specialist, or visit ibm.com/technology/cell/cell_hcls.html

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