Sales Guide:

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SGI Altix 450 Computational Chemistry Solution:

"The High-Performance Computational Chemist System"

Scientific Workflow Solution for Computational Chemistry:

SGI offers high-performance computing and storage solutions that address both specific computational chemistry workflows as well as multiple workflows that must be supported concurrently within a department. The Scientific Workflow Solution for Computational Chemistry is the conceptual umbrella that allows SGI to tailor specific implementations to meet the needs of individual customers. This solution provides the end-user with a single environment to both use computational resources and access data. It integrates Altix, Altix XE and InfiniteStorage NAS, SAN and Data Management capabilities in varying amounts depending on the customer's specific requirements.

Positioning:

If you are entering a new account, or are uncertain about the specific needs your customer is attempting to fill, you should lead with the high-level Scientific Workflow Solution for Computational Chemistry concept (Figure 1) and then refine your specific offering based on the specified customer requirements.

For most customers, a mix of Altix with Altix XE will deliver the best performance and price performance for the aggregate computational chemistry requirements. To determine the best mix, several key aspects of the customer environment have to be analyzed. These include:

Common User Environment		
Throughput Oriented And Small Problems	Flexible Mix of Large and Small Problems	Large Problems with Balanced Compute, Memory and I/O
SGI® Altix® XE • Small molecules ab initio Quantum Mechanics at low theory levels • Semi-Empirical Quantum Mechanics • Crystallography, Docking	SGI® Altix® and SGI® Altix® XE	SGI® Altix® • ab initio Quantum Mechanics • Plane Wave Quantum Mechanics • Larger Molecular Dynamics
SGI Storage, Archiving and Data Management Solutions NAS Servers, CXFS, DMF, Asset Management		
Common Management Environments Altair PBS Pro, Scali Manage, PCP, ESP		

Figure 1: Scientific Workflow Solution for Computational Chemistry

- The applications the customer is running. As noted in the Application Related Decision Criteria table, specific applications run better and/or scale better on one platform, so this is crucial.

- The number and size of problems. A customer with a few very large problems will likely benefit from Altix, while a customer with many smaller problems will benefit more from an Altix XE. For an individual research group, either large or small jobs may dominate, but for departments, a mix of job sizes is usually present.

- The need to focus. Customers that want to be able to focus all of their resources on specific high-priority problems will value the flexibility of the shared memory design of Altix. Customers that purchase point solutions will decide based on the ability of a platform to meet specific needs.

- The customer's system management capabilities and expertise with clusters. Managing a single Altix system is easier than managing multiple nodes in an Altix XE cluster. Customers with limited resources and/or cluster expertise may prefer an Altix system.

- Storage capacity, performance and archival requirements. SGI Altix systems require a single connection to storage and therefore are easier to deploy and can deliver higher I/O bandwidth. When compared to clusters, this is an added system management benefit for Altix users.

Altix 450 and Altix 4700 are critical parts of the SGI Workflow Solution for Computational Chemistry. They run key quantum mechanics code and scalable molecular mechanics/molecular dynamics applications extremely well. High CPU performance, scalability, dense packaging and attractive pricing make the Altix 450 the system of choice for research groups and departments.

Altix 450 Value Proposition for Computational Chemistry:

- SGI Altix 450 provides industry-leading per-CPU performance for the most demanding computational chemistry applications including Gaussian, VASP, CASTEP, and DMol3.

- SGI Altix provides leadership scalability that enables the solution of larger problems, and increases performance leadership.

- SGI Altix systems increase flexibility by being able to solve one large job, several medium jobs, many small jobs, or combinations of jobs.

- SGI Shared Memory systems simplify system management.

Application Related Decision Criteria

- Most computational chemistry departments run a mix of applications. The size of the problems being solved, the fit of applications to specific platforms, and the workload variation over time all need to be considered. Every customer will have a different set of specific requirements, but the following chart may be useful in determining the mix of Altix and Altix XE needed in a specific computing environment.

Applications	Fit with SGI Altix	Fit with SGI Altix XE Cluster	Notes
Quantum Mechanics: Plane Waves			
VASP, CASTEP Wien2K, CPMD	Overall: Very High CPU: High, heavy FP, optimized Scaling: High with SSI	Overall: Medium CPU: High with heavy FP Scaling: Medium with cluster	No native version of CASTEP on x86-64
Quantum Mechanics: ab initio			
Gaussian, DMol^3, Molpro	Overall: Very High CPU: High, heavy FP, optimized Scaling: High to Medium	Overall: Medium CPU: Medium Scaling: Medium to Low	Coding style favors Altix. Gaussian scales to ~2x CPUs on Altix than Altix XE
ADF, Jaguar, NWChem	Overall: High CPU: High, heavy FP Scaling: Medium	Overall: High CPU: High, heavy FP Scaling: Medium	NWChem is much more highly scalable than ADF & Jaguar
GAMESS	Overall: Medium CPU: Medium Scaling: High with SSI	Overall: Very High CPU: High, X86 optimized Scaling: Medium	Coding Style Favors Xeon CPUs, but Altix scales to ~2x CPUs
Quantum Mechanics: Semi-Empirical			
Mopac, Ampac, VAMP	Overall: Low CPU: Medium, mixed FP/Integer Scaling: Low – 4 CPUs	Overall: Medium to High CPU: Medium to high, benefits from clock speed Scaling: Low – 4 CPUs	Mostly small problems that run well in throughput mode on an Altix XE

Applications	Fit with SGI Altix	Fit with SGI Altix XE cluster	Notes
Molecular Mechanics / Molecular Dynamics			
Amber/PMEMD, NAMD, Discover	Overall: High CPU: High, mixed FP/Integer, some Itanium2 optimization Scaling: Very high on SSI	Overall: High CPU: High, mixed FP/Int, benefits from clock speed Scaling: High on clusters	Large to very large problems favor Altix
CHARMm, GROMACS	Overall: Medium CPU: Medium, mixed FP/Integer Scaling: Medium	Overall: High CPU: High, mixed FP/Int, benefits from clock speed Scaling: Medium-high	Coding style favors Altix XE, GROMACS uses special X86 instructions
Crystallography			
CNX, HKL, CCP4, ShelX	Overall: Low CPU: N/A Scaling: N/A	Overall: Very high CPU: High, mixed FP/Int, benefits from clock speed Scaling: Low (4 CPU) per job	Most Crystallography code only run on X86. Scaling comes from running many jobs simultaneously
Docking			
Dock, AutoDock, FlexX, Fred, Glide	Overall: Low CPU: N/A Scaling: N/A	Overall: Very high CPU: High, heavy integer, benefits from clock speed Scaling: Low (1 CPU) per job	Most Docking code only run on X86. Scaling comes from running many jobs simultaneously

Sample Solution Sizes and Options:

Altix 450 Solution Size	US Street Price	CPUs 1.6GHz 18M Cache	Memory	Disk	Service
Entry	$49,388	12	32GB	146GB SAS	1 year warranty
Mid	$99,128	24	64GB	292GB SAS	1 year warranty
High	$196,618	48	128GB	292GB SAS	1 year warranty
Small Storage	$19,363			3TB SAS	1 year warranty
Medium Storage	$47,153			8TB RAID	1 year warranty
Large Storage	$74,644			16TB RAID	1 year warranty

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