SGI® Altix® XE Servers and Clusters

Delivering Top Performance and Value for the Simplest to the Most Complex Workflows

The High-Throughput Computational Chemist System.

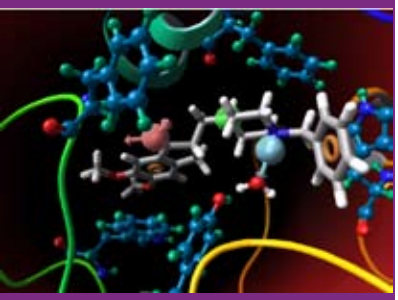


Image courtesy of Schrödinger.

The new SGI® Altix® XE server is the ideal high-throughput system to run a wide range of your critical Computational Chemistry applications, including the entire suite of Schrödinger software products. SGI Altix XE cluster systems provide industry leading high-throughput capability for semi-empirical quantum mechanics, small molecule ab initio molecular dynamics, crystallography, docking, and a wide range of additional computational chemistry applications. Many of these applications are optimized to run on X86-64 technology, and take advantage of the superior CPU performance and energy efficiency of the Intel Dual-Core Xeon 5100 series processors and Intel Quad-Core Xeon 5300 series processors.

Drive more results faster with your own Altix XE cluster. This fully factory integrated and tested configuration includes:

- One Altix XE 240 head node with two Intel® Quad-Core Xeon® 5300 Series processors (2.66GHz, 8MB on-die cache), 8GB memory, 500GB SATA HDD, DVD, 24-port Gigabit Ethernet switch, 1U slide-out console with keyboard and mouse, and 20U rack
- Five Altix XE 210 compute nodes (each with two quad-core Xeon processors, 8GB memory, and 500GB SATA HDD)
- Top performance with Dual- and Quad-Core Intel® Xeon® Processor-based server and cluster nodes
- Turbo-charged Computational Chemistry application performance with SGI® ProPack™ for Linux® OS
- Intel C++ and Fortran compilers, Intel Math Kernel Library, and Intel MPI
- Superior TCO with breakthrough energy efficiency (65 Watts/socket) and performance density (up to 16 processor cores per 1U chassis)
- Easy to build and deploy with custom-configurable, factory integrated clusters
- 1 Year of SGI warranty support
- Confidently backed 100% by SGI World-class Customer Service organization

Don't miss out on this special pricing… Please call 1-800-800-SGI1 (7441), e-mail at eleads@sgi.com, or contact your authorized SGI channel partner.

SGI® Altix® XE Servers and Clusters

Node Type
Altix XE210 and Altix XE240
- Head or Compute

Altix XE310
- Compute (two nodes per XE310)

Processors
Altix XE210 and Altix XE240
- Up to two Dual or Quad-Core Intel Itanium® Xeon® processors, 5100 Series or 5300 series

Altix XE310
- Up to four Dual or Quad-Core Intel Itanium® Xeon® processors, 5100 Series or 5300 series (two per node)
- Compute (two nodes per XE310)
- Front Side Bus: 1333 or 1066MHz
- CPU clock rates: 3.0, 2.66, 2.33, or 2.0GHz
- L2 Cache: 4.0MB for Dual-Core, 8.0MB for Quad-Core

Memory
Altix XE210 and Altix XE240
- 32GB DDR2 667MHz FBDIMM memory

Altix XE310
- 64GB DDR2 667MHz FBDIMM memory (32GB per node)

Integrated I/O
Altix XE210 and Altix XE240
- 16MB ATI (ES1000) graphics
- 1 x RJ45 Serial B port on rear
- 3 x USB 2.0 port; 1 front, 2 rear
- PS/2 Keyboard & Mouse ports
- 2 x RJ45 10/100/1G Ethernet (Intel® 82563EB)

Altix XE310
- 2 x InfiniBand Port (1 per node), optional
- 2 x COM port (1 per node)
- 2 x VGA (1 per node)
- 2 x Gigabit Ethernet (1 per node)
- 2 x USB ports (1 per node)

PCI Slots
Altix XE210
- 1 x PCIe x8 (low profile)
- 1 x PCI-X 133MHz (full height)

Altix XE240

Option 1:
- 2 x PCIe x4 (low profile)
- 2 x PCIe x4 (full height) or 1 x PCEe x8 (full height)
- 1 x PCI-X 133MHz (full height)

Option 2:
- 2 x PCIe x4 (low profile)
- 3 x PCI-X 133MHz (full height)

Altix XE310
- 2 x PCIe x8 (1 per node)

Internal Storage
Altix XE210
- Three SATA/SAS drive bays

Altix XE240
- Five SATA/SAS drive bays

Altix XE310
- Four SATA drive bays (two per node)
- 3.5" SATA drive: 250GB/7200 rpm; 500GB/7200 rpm
- 3.5" SAS drive: 73GB/15000 rpm; 146GB/10000 rpm
- 1 x DVD-ROM drive

Cluster Interconnects
Altix XE210 and Altix XE240
- InfiniBand and/or Gigaband Ethernet
- PCI-X and PCI-Express SDR and DDR InfiniBand HCAs
- One external Gigabit Ethernet port

Altix XE310
- InfiniBand and/or Gigaband Ethernet
- Two external 4X DDR InfiniBand port (optional; 1 per node)
- Two external Gigabit Ethernet ports (1 per node)

External Storage
- SGI InfiniteStorage Series; StorageTek® Tape Libraries; IBM 3590, LTO-2, LTO-3; HP® LTO-2, LTO-3; Quantum® SDLT, SDLT 220/320, SDLT 600; Sony® AIT-3, SAIT, DTF

Software
System Software
- Novell SUSE™ Linux Enterprise Server
- Red Hat® Enterprise Linux®
- SGI® ProPack™ for Linux® OS
- Microsoft® Windows® Compute Cluster Server

Software Solution Stack
- **Cluster Management Software:** Scali Manage
- **Job Scheduling / Workload Management:** Altair® PBS Professional™
- **Interconnect Fabric Management:** Voltaire GridStack
- **Filesystem:** XFS™ 64-bit journaled filesystem (avail. on SUSE Linux OS), CXFS™ shared filesystem for SANs
- **Network Filesystem:** Samba®

Development Tools
- Programming Languages, Compilers, Debuggers, Libraries, Parallel Programming, Performance Analysis
- For more details, see the SGI® Altix® XE Datasheet

Electrical and Power Supply
Altix XE210 and Altix XE240

1U Chassis
- One 600W power supply.

2U Chassis
- One 750W power supply with an optional redundant 750W power supply.

Voltage
- 200-240 VAC (North America/Japan)
- 230 VAC (International)

Power Requirements (max.)
- Short rack: 3.36 kW
- Tall rack: 7.20 kW

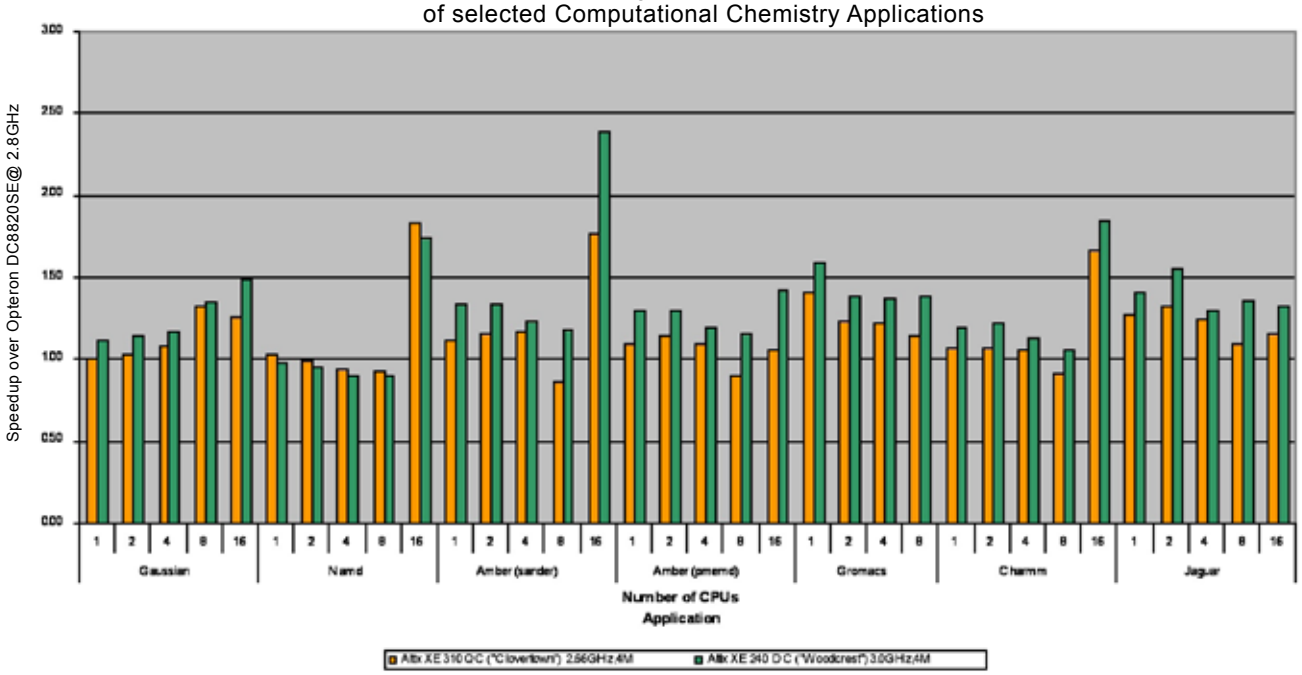
Altix XE310
- One 980W power supply.

Voltage
- 200-240 VAC (North America/Japan)
- 200-240 VAC (International)

Power Requirements (max.)
- Short rack: 8 kW
- Tall rack: 32 kW

Support and Services
SGI provides support for hardware and systems software. SGI offers services to implement and integrate Linux applications in your environment. SGI also offers SGI ESP (Embedded Support Partner), a set of tools and facilities that provides an effective, reliable, proactive, and automated environment for achieving levels of high availability. For more information, please see www.sgi.com/support or contact your SGI representative.

Average Relative speed
of selected Computational Chemistry Applications



Notes:
All performance results reported as the sum of all the times normalized by the total time of the reference machine. All testing done by SGI. SGI Altix 450 system tested: dual-core Intel Itanium 2 9040 (1.6GHz/18MB L3 cache per socket), 8 blades, 16 sockets, 32 cores, 64GB mem (2GB mem/core). SGI Altix XE 310 Quad-Core system tested: quad-core Intel Xeon 5300 (2.66GHz/8MB cache per socket), 2 sockets, 8 cores, 16GB mem. SGI Altix XE 240 Dual-Core system tested: dual-core Intel Xeon 5160 (3.0GHz/4MB cache per socket), 2 sockets, 4 cores, 8GB mem. Colfax DC 8220 system tested: dual-core AMD Opteron 8220SE (2.8GHz/2MB L2 cache per socket), 4 sockets, 8 cores, 32GB mem. Interconnect InfiniBand. Gaussian 03 rev D.01. Testing based on apinefreq (C10H16, 182 basis functions, RB3LYP/6-31G, Frequency calculation), apinenehf (C10H16, HF/6-311g(df,p), 346 basis functions), 1est397 (RB3LYP/3-21G Force calculation of C54H90N6O18, C1 symmetry, 882 basis functions.), TATBcis (CIS=Direct, SCF=Nolncore calculation of C6H6N6O6, C2v symmetry, 6-311g(2d,p) basis set, 171 basis functions). Amber 9. Testing based on jac, factor_ix, hb, rt, trx, gb_alp, gb_cox2 and gb_mb (http://amber.scripps.edu/). Namd 2.6. Testing based on apoa1 (http://www.ks.uiuc.edu/Research/namd/performance.html) and JAC. Charmm c33b1. Testing based on JAC and MbCOdyn (Carobxymyoglobin Dynamics 1,000 steps (1 ps) Number of Atoms: 17,491 (4,985 waters), 12A cutoff + PME. Gromacs 3.3.1. Testing based on villin, Lys/cut, Lys/PME, dppc and poly-ch2 (http://www.gromacs.org/content/view/24/37/). Jaguar 7.0.105. Tsting based on cholesterol - b3lyp/pvtz ("One step of Geometry optimization of Cholesterol (C27H46O; C1 symmetry) b3lyp, cc-pvtz(-f) basis set, 74 atoms, 1058 basis functions"), taxol b3lyp/6-31g (One step of Geometry optimization of Taxol (C47NH51O14; C1 symmetry), b3lyp, 6-31g** basis set, 113 atoms, 1185 basis functions); mimic -lmp2/pvtz (LMP2 calculation (C12H14O3F2; C1 symmetry), cc-pvtz basis set, 31 atoms, 706 basis functions); cholesterol - lmp2/6-31g ("LMP2 calculation of Cholesterol (C27H46O; C1 symmetry) 6-31g** basis set, 74 atoms, 650 basis functions); cholesterol - lmp2/pvtz ("LMP2 calculation of Cholesterol (C27H46O; C1 symmetry) cc-pvtz(-f) basis set, 74 atoms, 1058 basis functions); dioxin -freq-6-31g ("Frequency calculation of dioxin(C12H4Cl4O2; D2h symmetry) b3lyp, 6-31g** basis set, 22 atoms, 306 basis functions); tetramethrin lmp2-cc-pvtz(-f) ("LMP2 calculation of tetramethrin (C19NH25O4; C1 symmetry) cc-pvtz(-f) basis set, 49 atoms, 777 basis functions); "emetine - freq-631g ("Frequency calculation of emetine (C27N2H36O4; C1 symmetry) b3lyp, 6-31g** basis set, 69 atoms, 675 basis functions). Detailed performance results are available upon request.

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