



Guvernul
Romaniei

Proiect CAPACITATI

Modernizarea Departamentului de Fizica Moleculara si Biomoleculara



Institutul National de Cercetare-Dezvoltare pentru
Tehnologii Izotopice si Moleculare – Cluj Napoca

ANCS
Autoritatea Națională pentru Cercetare Științifică

www.itim-cj.ro/mdfmolbio

Denumirea Investitiei :

Stație de lucru pentru calcul de înaltă performanță

Valoarea estimata : aprox. 300 mii EURO
Data achizitionarii : Noiembrie 2011

Performante Tehnice



Graphics Cards

- 2D Card: ATI™ FireMV 2200 PCI Low Profile, Max analog resolution 2048 x 1536, 64MB memory
- 3D Card: ATI FireGL V7350 PCI-E, Max digital resolution 3840 x 2400, 1GB memory
- SUSE Linux Enterprise Server

SGI® RASC™ Blade

- Two high performance Xilinx Virtex 4 LX200 FPGA chips with 160K logic cells
- 10 QDR SRAM DIMMs per blade
- SUSE Linux Enterprise Server

External Storage Options

JBOD

- SGI® InfiniteStorage 120

RAID

- SGI® InfiniteStorage 4000, 4500, 6700, 10000

NAS and SAN Solutions

- SGI® InfiniteStorage 2000, 3000

Tape and Libraries - Many Options Available

Software

Operating System

- SUSE Linux Enterprise Server
- Red Hat Enterprise Linux Advanced Server
- Optional SGI® ProPack™ on SUSE® Linux Enterprise Server

Host Storage Software

- XVM, XVM Ple, XVM Snapshot, XFS®, CXFS™, DMF, InfiniteStorage Resource Manager

Networking

- TCP/IP, NFS V2/V3, DHCP, SNMP management, SNMP MIB, NIS/ONC+

Software Development Tools

Compilers

- Intel C++ and Fortran Compilers for Linux
- GNU Compiler for C and Fortran 77

Libraries

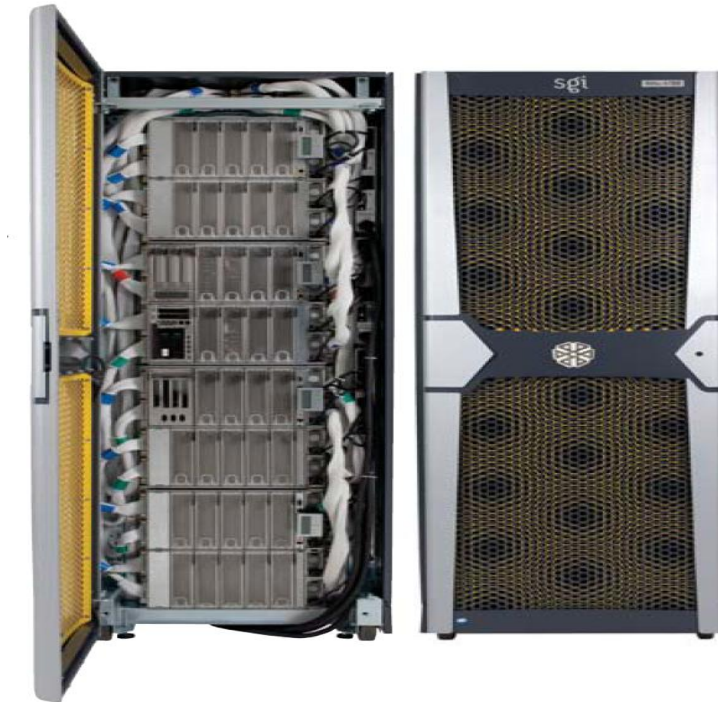
- SGI Message Passing Toolkit (MPT)
- Intel MPI and Math Kernel Libraries
- SGI Flexible File Input/Output (FFIO)
- Intel Integrated Performance Primitives (Intel IPP)

Debuggers

- Intel Debugger
- Etnus® TotalView®
- GNU GDB
- Alinea Software Distributed Debugging Tool (DDT)

Analysis Tools

- Intel VTune™ Performance Analyzer
- Intel Trace Analyzer and Intel Trace Collector
- SGI Performance Co-Pilot™



- OpenMP: OpenMP included w/Intel compilers
- Parallel Software Products ParaWise

Open Source Development Tools

- Linuxapps, Freshmeat

FPGA Software Development Tool

- SGI's FPGA-aware gdb
- HLL tools: Mitronics MitronC, Celoxica Handel-C and DK Design Suite

Threading Tools

- Intel Thread Checker
- Intel Threading Building Blocks

Dimensions and Weight

Individual Rack Unit (IRU)

- Supports up to 10 blade slots
- 10U (17.38"H x 17.5"W x 32.5"D)
- Maximum weight: 263 Lbs (119kg)

Standard Rack

- Four IRU per rack
- 42U (79.5"H x 25.6"W x 45.0"D)
- Maximum weight: 1450 lbs (668kg)
- Lockable front and rear

Compute Blades

Density Configuration

Two processor sockets per blade

- Up to 78* Intel® Itanium® Processor sockets per rack
- Dual Core Intel® Itanium® Series 9000 1.67GHz, 8, 18 or 24MB/667MHz FSB
- 8 DIMM slots per blade: 1GB, 2GB or 4GB DIMMs

Bandwidth Configuration

One processor socket per blade

- Up to 39* Intel® Itanium® Processor sockets per rack
- Dual-Core Intel® Itanium® Series 9000 1.67GHz, 8, 18 or 24MB/667MHz FSB
- 8 DIMM slots per blade: 1GB, 2GB or 4GB DIMMs

Memory-only Blade

- Adds to shared memory without cost of cpu and associated software licenses
- 12 DIMM slots per blade: 1GB, 2GB or 4GB DIMMs



DatacenterBlade™

DatacenterBlade™ (SBE-714D-R42/D28) is perfect for data center and HPC applications with performance & density optimized to achieve 672 processing cores and 4TB DDR2 memory per 42U standard rack. This powerful SuperBlade® features 100-240VAC, ultra high-efficiency (93%), N+1 redundant power supplies, along with industry-leading density, performance/watt and price/performance.

DatacenterBlade™ Features:

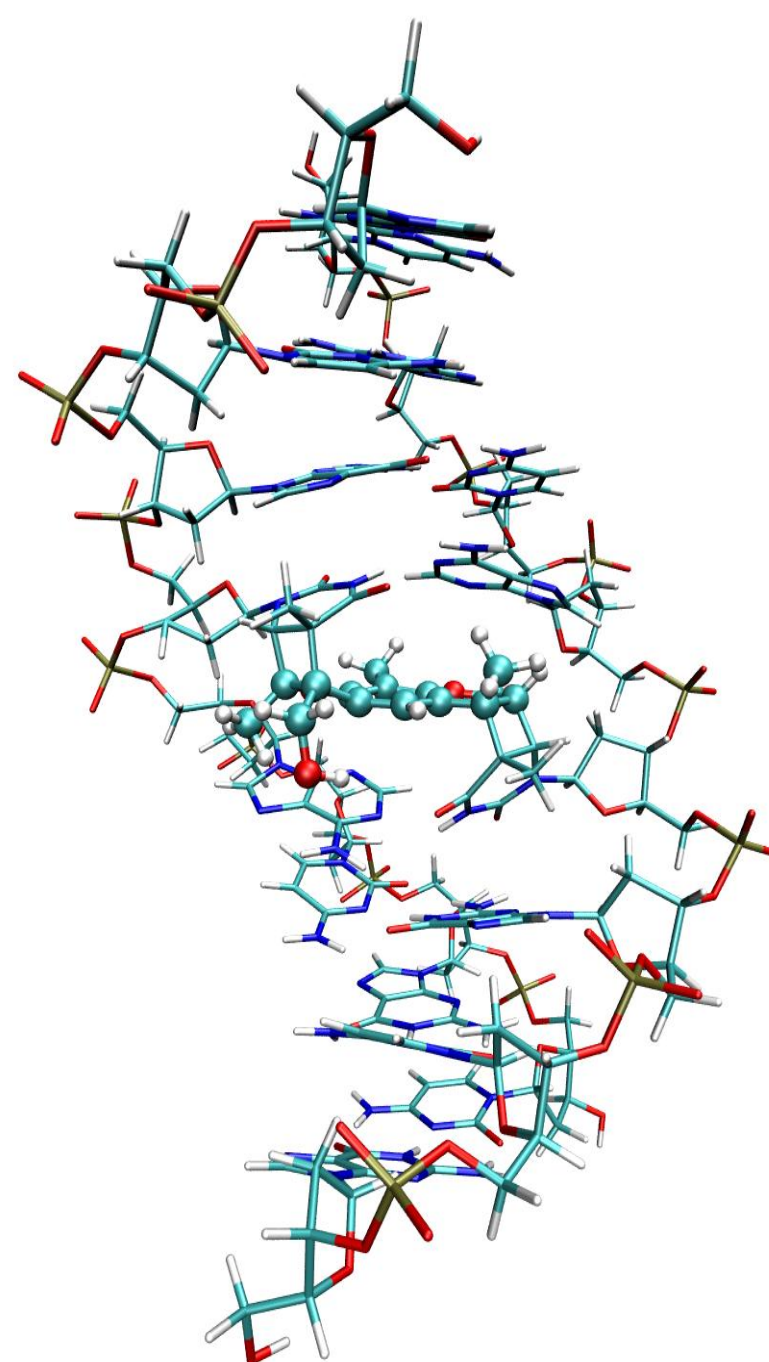
- High density – 14 DP blades in 7U enclosure; up to 672 processing cores in standard 42U rack
- High performance – up to 0.27 GFlops/watt *
- Energy efficiency – 93% efficiency power supplies and native DDR2 memory instead of FBD memory
- High availability – N+1 redundant power supplies
- Ease of Use – easy to set up with remote management tools
- Flexibility – two or four 100-240VAC power supplies
- High-performance storage – 3x SAS/SATA drives per server blade with RAID 0, 1, 5, 10

DatacenterBlade™ Benefits:

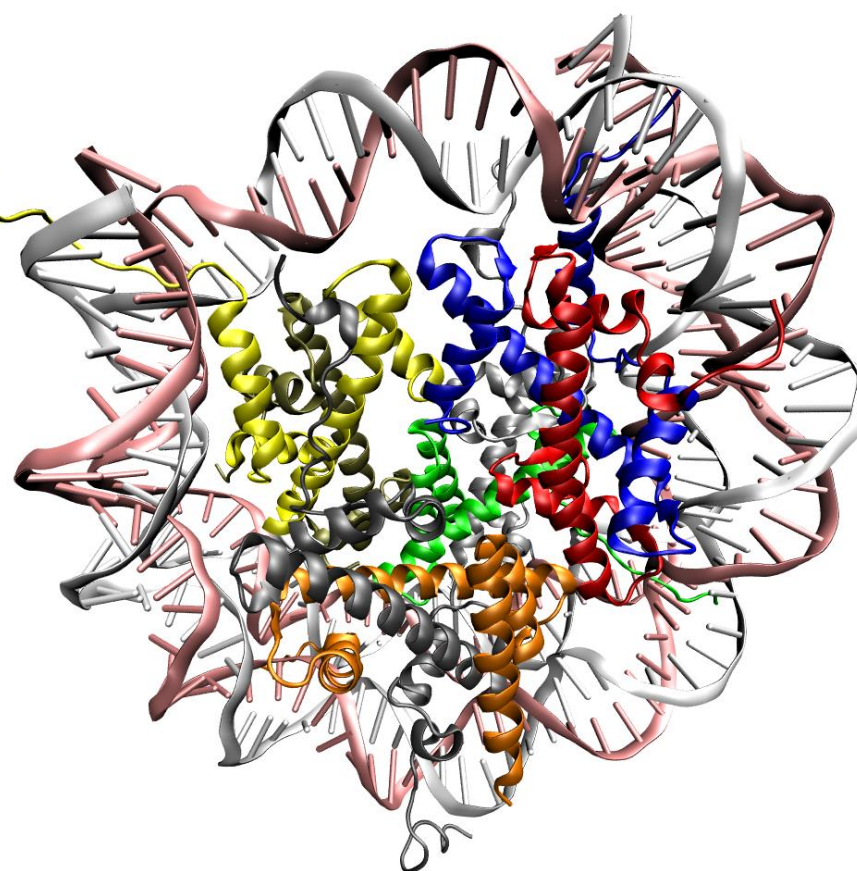
- Industry-leading performance/watt – best for data center applications
- Ultra-high power efficiency – energy savings
- High performance, high availability, high density
- Industry-leading price/performance

Server Module	Processor(s)	Cores/Threads	Memory Capacity
Sun Blade X8400 server module	4 dual-core AMD Opteron Series 800 processors	• 2 cores, 2 threads	Up to 64 GB, 16 DIMM slots
Sun Blade X8420	4 dual-core AMD Opteron Series 8000 processors	• 2 cores, 2 threads	Up to 64 GB, 16 DIMM slots
Sun Blade X8440 server module	2 or 4 second- or third-generation AMD Opteron processors	• Second generation: 2 cores, 2 threads • Third generation: 4 cores, 4 threads	Up to 128 GB, 32 DDR2 DIMM slots
Sun Blade X8450 server module	2 or 4 Intel Xeon Processor 7200 series or 7300 series processors	• 7200 series: 2 cores, 2 threads • 7300 series: 4 cores, 4 threads	Up to 128 GB, 32 FB-DIMM slots

Aplicatii Practice



- Interacții moleculare;
- Sisteme moleculare autoasamblate;
- Efecte de intercalare în ADN, prototipul interacției molecula medicament – bio-moleculă;
- Interacții moleculă – suprafață metalică;
- Efecte de agregare moleculară;
- Procese de incluziune moleculară: gazdă – oaspete;
- Modelări de spectre IR, Raman și RMN;
- Excitări moleculare, procese non-adiabactice;
- Interacția câmpului electromagnetic (câmp laser) cu sisteme moleculare;
- Conductibilitatea purtătorilor de sarcini în sisteme biomoleculare;



- Colaborări cu instituții, universități și centre academice din țară și din străinătate;
- Realizarea unor proiecte de cercetare complexe având ca parteneri și companii private;
- Obținerea unor produse bazată pe tehnologie moleculară: biosensori, materiale moleculare cu proprietăți specifice sau funcționalizate;

