

Materials Studio 5.0 System Requirements

Supported Clients

Note. For Windows Clients and Servers, only the 32-bit version of the operating system is supported.

Supported Clients

Operating Systems

- Windows XP Professional SP3
- Windows Vista SP2:
 - Enterprise
 - Business

Supported Servers

[View supported servers for each Materials Studio module »](#)

Operating Systems

- Windows XP Professional SP3
- Windows Server 2003 SP2 and R2:
 - Web
 - Standard
 - Enterprise
 - Datacenter
- Windows Server 2008 SP2
 - Web
 - Standard
 - Enterprise
 - Datacenter
- Windows Vista SP2:
 - Enterprise
 - Business

- Red Hat Enterprise Linux WS, ES and AS 4.7 and 4.8 on x86 and x86-64 processors and clusters thereof
- Red Hat Enterprise Linux 5.3 and 5.4 and Desktop 5.3 and 5.4 on x86-64 processors and clusters thereof
- Red Hat Enterprise Linux 5.3 and 5.4 on Itanium processors
- SuSE Linux Enterprise Server 10 (SP1 & SP2) on x86 and x86-64 processors
- SuSE Linux Enterprise Server 11 on x86-64 processors
- SuSE Linux Enterprise Server 10 (SP1 & SP2) on Itanium processors, for standalone execution of CASTEP, DMol³ and Discover only (no gateway support) .
- SuSE Linux Enterprise Server 11 on Itanium processors, for standalone execution of CASTEP, DMol³ and Discover only (no gateway support) .

In general, all of the supported server configurations listed above can be used to run selective executables in parallel - these include CASTEP, DMol³, Discover, Forcite Plus, ONETEP, GULP, MesoDyn, and Mesocite. Installation of the MPI runtime environment, HP-MPI, is platform dependent:

- On Windows, HP-MPI is installed as part of the Materials Studio installation process
- On Linux, HP-MPI must be installed before Materials Studio. It is provided on the Unix Installers DVD.

Note. Platform Computing has acquired HP-MPI. This is now commercially available as Platform MPI 7 but the version of MPI supplied with Materials Studio 5.0 is still referred to as HP-MPI.

The [platform matrix](#) contains a summary of supported server platforms.

Queuing Systems

In general, submission of serial jobs from the Materials Studio client to servers running PBS, or LSF queuing systems is supported. The software has been tested against the following versions of queuing systems:

- PBS Pro 10.1 on all systems
- LSF v7.0 Update 5
- Sun Grid Engine (SGE) 6.2

Restrictions

- In general, support is certified only for serial jobs on queuing systems serving single machines
- For parallel execution, CASTEP, DMol³, Discover, Forcite Plus, ONETEP, GULP, MesoDyn, and Mesocite MPI versions are supported for submission on Linux clusters and SMP machines running PBS Pro, LSF, and Sun Grid Engine

- PBS Pro on Windows is not supported for MPI parallel jobs.

Recommended Hardware

Clients

The minimum recommended configuration for running Materials Studio is as follows:

- Intel Pentium® 4 or compatible processor running at 1GHz
- Standard Microsoft 2-button mouse
- 1024 x 768 minimum display resolution
- 1GB RAM
- 16 bit or 65536 colors
- A maximum of 730MB disk space for an install of all components (client and server)

Servers

Windows

- Intel Pentium® 4 or compatible processor running at 1Ghz
- 1GB RAM
- A maximum of 1GB disk space for an install of all components

LINUX x86 and x86-64 PCs

- Intel Pentium® 4 or compatible processor running at 1GHz
- 1GB RAM
- A maximum of 1GB disk space for an install of all components

LINUX x86 and x86-64 Clusters

- Intel Pentium® 4 or compatible processors running at 1GHz or greater
- 1GB RAM per node
- Up to 16 processor cores per job, we recommend one or two processor cores per node
- Only homogeneous clusters (identical processors, identical OS, libraries, *etc.* on each node)
- 1 GB disk space per node
- All interconnects supported by HP-MPI. We have certified support only for Gigabit Ethernet, Infiniband interconnects and for Myrinet switches, although other interconnects should work if supported by HP-MPI. For MPI-parallel Materials Studio applications that are only supplied as 32-bit binaries (MesoDyn), when running on Opteron or EM64T platforms, TCP will be used on the IB and Elan interconnects. Note that some Infiniband Drivers work only with Linux kernel versions 2.6.16 (included with Redhat 5) or higher and HP-MPI 2.2.7 and higher.

- Beowulf architecture, with a head node that holds the file system, Materials Studio installation, and user data. These files must be mounted and visible to the compute nodes at the same location as on the head node.
- Compute nodes must be able to communicate with each other and the head node via rsh or ssh, without password (for MPI).
- License file or license server must be installed on the head node, unless the compute nodes are configured so they can see the license server elsewhere.
- HP-MPI should be installed as part of the software installation, so there are no specific further requirements. In general, HP-MPI must be installed on each cluster node individually.
- Currently only DMol3, CASTEP, Discover, ONETEP, Forcite Plus, GULP, Mesodyn and Mesocite servers are supported for parallel execution on Linux clusters.
- For serial operation, all server codes are supported on Linux clusters, provided the queuing systems PBS Pro, SGE, or LSF are installed on the cluster to distribute such serial jobs over the compute nodes.

LINUX IA64 Workstations

- A maximum of 730MB disk space for an install of all components per node
- Note that support for the SuSE Linux option is limited to CASTEP, DMol³, and Discover.

HP XC clusters running LINUX

- At least 730MB disk space for an install of all components per node, plus ample disk space on the head node for files generated by running jobs. Some parallel applications also require substantial temporary disk space on the compute nodes.
- HP Cluster Platform 3000, HP Cluster Platform 4000, HP Cluster Platform 6000.
- All interconnects supported by HP-MPI. We have certified support only for Gigabit Ethernet, Infiniband interconnects and for Myrinet switches, although other interconnects should work if supported by HP-MPI.
- For MPI parallel Materials Studio applications that are only supplied as 32-bit binaries (MesoDyn), when running on Opteron or EM64T platforms, TCP will be used on the IB and Elan interconnects.
- The head node should hold the file system, Materials Studio installation, and user data. These files must be mounted and be visible to the compute nodes at the same location as on the head node.
- Compute nodes must be able to communicate with each other and the head node via ssh, without password (for MPI).
- License file or license server must be installed on the head node, unless the compute nodes are configured so they can see the license server elsewhere.
- HP-MPI is pre-installed on the XC cluster.

- Currently only DMol³, CASTEP, Discover, Forcite Plus, ONETEP, GULP, MesoDyn, and Mesocite servers are supported for parallel execution on XC clusters.
- For serial operation, other server codes are supported on XC clusters through the LSF queuing system.
- XC system software 4.0 or higher