



# **SYSTEM REQUIREMENTS** MATERIALS STUDIO 2023



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#### Third Party Notification

Your BIOVIA Materials Studio 2023 installation contains third-party software components. For details, refer to the BIOVIA Program Directory at <a href="https://media.3ds.com/support/progdir/">https://media.3ds.com/support/progdir/</a>.

#### Acknowledgments and References

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# **About This Document**

This documents the details of the system requirements for Materials Studio 2023 client and server. For installation instructions, refer to the *Materials Studio 2023 Installation and Administration Guide*.

# Definitions

The following defines specific terms for BIOVIA Materials Studio 2023:

- Supported: The hardware or software was tested against BIOVIA Materials Studio, is expected to
  function as documented, and will be supported by BIOVIA. If issues are found that are specific to
  these versions of the hardware or software, they will be addressed in accordance with the BIOVIA
  software support policy.
- Not Supported: Any hardware and software not specifically listed in this document is not supported by BIOVIA. These are used at the customer's risk and BIOVIA makes no guarantee regarding the capability of unsupported hardware or software to function with BIOVIA Materials Studio.
- Known to Be Incompatible: Software, or versions of software, that will not function correctly in conjunction with BIOVIA Materials Studio 2023.
- Regional Language Settings: The ability to change the format that Microsoft<sup>®</sup> Windows uses to display dates, times, large numbers and decimal fractions. This document includes the regional language settings that BIOVIA supports for BIOVIA Materials Studio.

# **Materials Visualizer Requirements**

This section describes the requirements of the Materials Visualizer *only*. The Materials Visualizer is the core client module in Materials Studio; providing modeling, analysis, and visualization tools. It cannot set up or launch jobs *unless* installed in conjunction with Materials Studio Server.

# **Supported Operating Systems**

Operating System	Supported Versions	Notes
Microsoft Windows Professional & Enterprise	10	64-bit only
	11	

# **Hardware Requirements**

Component	Minimum Hardware	Recommended
Processor	Intel <sup>®</sup> Core™ i5 or equivalent	Intel Core i7 or equivalent
RAM	4 GB	16 GB
Available hard disk space	1 GB	4 GB
for installation	The hard disk space required for insta Materials Visualizer only and 4 GB if y Studio server and client. The Materia on Windows. Additional space will be necessary, for example for .NET, runt	allation can vary between 1 GB for ou install the complete Materials Is Visualizer can only be installed required if system updates are imes, and libraries.
Display	1366 × 768 display resolution 24-bit	1920 × 1080 display resolution 32-bit

If you are installing the Materials Visualizer and Materials Studio server on the same machine, it should satisfy the <u>minimum server requirements</u>.

### **Browsers**

The following browsers are supported on client operating systems:

- Microsoft Edge, 64-bit
- Mozilla Firefox ESR, 64-bit and 32-bit compatible
- Google Chrome, 64-bit

# **Materials Studio Server Requirements**

This section describes the requirements of the Materials Studio Server only.

## **Supported Operating Systems**

Only 64-bit server operating systems are supported.

Operating System	Versions	Notes
Microsoft Windows Professional & Enterprise	10 11	
Microsoft Windows Server Standard & Datacenter	2016 2019 2022	
Red Hat Enterprise Linux	7.5, 7.6, 7.7, 7.8, 7.9 8.2, 8.3, 8.4, 8.5, 8.6	
CentOS	7.5, 7.6, 7.7, 7.8, 7.9	8.x versions are no longer supported.

**Note:** If you intend to run server applications in parallel on a Windows system that does not have a network connection, you should install the Microsoft Loopback Adapter by following instructions appropriate to your operating system.

### **Hardware Requirements**

Component	Minimum Hardware	Recommended
Processor	Intel <sup>®</sup> Xeon <sup>®</sup> E5-1620 or equivalent	Intel Xeon Silver 41XX series or equivalent
RAM per core (at least two cores)	2 GB	8 GB
Available hard disk space	4 GB	4 GB
for installation	The hard disk space required for installation can vary between 1 GB for Materials Visualizer only and 4 GB if you install the complete Materials Studio server and client. The Materials Visualizer can only be installed on Windows. Additional space will be required if system updates are necessary, for example for .NET, runtimes, and libraries.	

Greater processing power and memory are recommended for any heavy-duty use.

As you use Materials Studio to create structures, run calculations, gather and analyze results, the disk space required increases for storage of both results and interim job files on the server. Ensure that the server you use for Materials Studio has enough disk space to accommodate your long-term space requirements.

See the <u>Materials Visualizer Requirements</u> section for further recommendations to help you get the best out of Materials Studio visualization. There are no graphics-related requirements for running Materials Studio on Windows servers.

### **GPU Support**

Materials Studio supports calculations on a single GPU on 64-bit Linux and Windows servers. The GPU must conform to these requirements:

- NVIDIA cards
- Support for Compute Capability 6.0 or higher with CUDA version 10.1

**Tip:** Ensure that you have installed an up-to-date version of the driver provided by NVIDIA for your graphics card.

### **Linux Server System Libraries**

On Linux systems, Materials Studio requires the standard C++ libraries for backward compatibility of the C++ compiler for proper operation of the server codes. Install these libraries before installing Materials Studio and BIOVIA License Pack.

These lists detail the packages that contain the required libraries for the two most recent OS minor supported versions at the time of Materials Studio release.

**Note:** Libraries marked \* are required for a root RPM installation.

If you have a newer version of a package than those listed, then no action should be required.

#### **Red Hat Enterprise Linux 7.8**

- audit-libs-2.8.5-4.el7.x86\_64
- bzip2-libs-1.0.6-13.el7.x86\_64
- fontconfig-2.13.0-4.3.el7.x86\_64
- freetype-2.8-14.el7 9.1.x86 64
- glibc-2.17-307.el7.1.x86\_64
- keyutils-libs-1.5.8-3.el7.x86 64
- krb5-libs-1.15.1-46.el7.x86\_64
- libcap-ng-0.7.5-4.el7.x86\_64
- libcom err-1.42.9-17.el7.x86 64
- libgcc-4.8.5-39.el7.x86\_64
- libpng-1.5.13-7.el7\_2.x86\_64
- libselinux-2.5-15.el7.x86 64

- libstdc++-4.8.5-39.el7.x86\_64
- libuuid-2.23.2-63.el7.x86\_64
- libX11-1.6.7-4.el7 9.x86 64
- libXau-1.0.8-2.1.el7.x86 64
- libxcb-1.13-1.el7.x86\_64
- libXext-1.3.3-3.el7.x86\_64
- libXrender-0.9.10-1.el7.x86\_64
- nss-softokn-freebl-3.67.0-3.el7\_9.x86\_64
- pam-1.1.8-23.el7.x86\_64
- zlib-1.2.7-20.el7\_9.x86\_64
- redhat-lsb-core-4.1-27.el7.x86\_64
- shadow-utils-4.6-5.el7.x86\_64

# Red Hat Enterprise Linux 7.9

- audit-libs-2.8.5-4.el7.x86 64
- bzip2-libs-1.0.6-13.el7.x86 64
- fontconfig-2.13.0-4.3.el7.x86 64
- freetype-2.8-14.el7\_9.1.x86\_64
- glibc-2.17-326.el7 9.x86 64
- keyutils-libs-1.5.8-3.el7.x86 64
- krb5-libs-1.15.1-54.el7\_9.x86\_64
- libcap-ng-0.7.5-4.el7.x86 64
- libcom err-1.42.9-19.el7.x86 64
- libgcc-4.8.5-44.el7.x86 64
- libpng-1.5.13-8.el7.x86\_64
- libselinux-2.5-15.el7.x86\_64

# Red Hat Enterprise Linux 8.5

- audit-libs-3.0-0.17.20191104git1c2f876.el8.x86\_64
- bzip2-libs-1.0.6-26.el8.x86\_64
- compat-openssl10-1.0.2o-3.el8.x86 64
- fontconfig-2.13.1-4.el8.x86\_64
- freetype-2.9.1-4.el8\_3.1.x86\_64
- glibc-2.28-164.el8.x86\_64
- keyutils-libs-1.5.10-9.el8.x86\_64
- krb5-libs-1.18.2-14.el8.x86\_64
- libcap-ng-0.7.11-1.el8.x86\_64
- libcom\_err-1.45.6-2.el8.x86\_64
- libgcc-8.5.0-3.el8.x86\_64
- libnsl-2.28-164.el8.x86\_64
- libpng-1.6.34-5.el8.x86\_64
- libselinux-2.9-5.el8.x86 64

- libstdc++-4.8.5-44.el7.x86 64
- libuuid-2.23.2-65.el7 9.1.x86 64
- libX11-1.6.7-4.el7\_9.x86\_64
- libXau-1.0.8-2.1.el7.x86 64
- libxcb-1.13-1.el7.x86 64
- libXext-1.3.3-3.el7.x86 64
- libXrender-0.9.10-1.el7.x86 64
- nss-softokn-freebl-3.67.0-3.el7\_9.x86\_64
- pam-1.1.8-23.el7.x86 64
- zlib-1.2.7-20.el7\_9.x86\_64
- redhat-lsb-core-4.1-27.el7.x86 64 \*
- - libstdc++-8.5.0-3.el8.x86\_64
  - libuuid-2.32.1-28.el8.x86 64
  - libX11-1.6.8-5.el8.x86 64
  - libXau-1.0.9-3.el8.x86\_64
  - libxcb-1.13.1-1.el8.x86\_64
  - libxcrypt-4.1.1-6.el8.x86\_64
  - libXext-1.3.4-1.el8.x86\_64
  - libXrender-0.9.10-7.el8.x86\_64
  - openssl-libs-1.1.1k-7.el8\_6.x86\_64
  - pam-1.3.1-15.el8.x86\_64
  - pcre2-10.32-2.el8.x86\_64
  - zlib-1.2.11-18.el8\_5.x86\_64
  - redhat-lsb-core-4.1-47.el8.x86 64 \*
  - shadow-utils-4.6-14.el8.x86 64 \*

- - - shadow-utils-4.6-5.el7.x86\_64 \*

#### **Red Hat Enterprise Linux 8.6**

- audit-libs-3.0.7-2.el8.2.x86\_64
- bzip2-libs-1.0.6-26.el8.x86\_64
- compat-openssl10-1.0.2o-4.el8\_6.x86\_64
- fontconfig-2.13.1-4.el8.x86\_64
- freetype-2.9.1-4.el8\_3.1.x86\_64
- glibc-2.28-189.5.el8\_6.x86\_64
- keyutils-libs-1.5.10-9.el8.x86\_64
- krb5-libs-1.18.2-14.el8.x86\_64
- libcap-ng-0.7.11-1.el8.x86\_64
- libcom\_err-1.45.6-4.el8.x86\_64
- libgcc-8.5.0-10.1.el8\_6.x86\_64
- libnsl-2.28-189.5.el8\_6.x86\_64
- libpng-1.6.34-5.el8.x86\_64
- libselinux-2.9-5.el8.x86\_64

#### CentOS Linux release 7.8.2003

- audit-libs-2.8.5-4.el7.x86\_64
- bzip2-libs-1.0.6-13.el7.x86\_64
- fontconfig-2.13.0-4.3.el7.x86\_64
- freetype-2.8-14.el7\_9.1.x86\_64
- glibc-2.17-307.el7.1.x86\_64
- keyutils-libs-1.5.8-3.el7.x86\_64
- krb5-libs-1.15.1-46.el7.x86\_64
- libcap-ng-0.7.5-4.el7.x86\_64
- libcom\_err-1.42.9-17.el7.x86\_64
- libgcc-4.8.5-39.el7.x86\_64
- libpng-1.5.13-7.el7\_2.x86\_64
- libselinux-2.5-15.el7.x86\_64

- libstdc++-8.5.0-10.1.el8\_6.x86\_64
- libuuid-2.32.1-35.el8.x86\_64
- libX11-1.6.8-5.el8.x86\_64
- libXau-1.0.9-3.el8.x86\_64
- libxcb-1.13.1-1.el8.x86\_64
- libxcrypt-4.1.1-6.el8.x86\_64
- libXext-1.3.4-1.el8.x86\_64
- libXrender-0.9.10-7.el8.x86\_64
- openssl-libs-1.1.1k-7.el8\_6.x86\_64
- pam-1.3.1-16.el8.x86\_64
- pcre2-10.32-3.el8\_6.x86\_64
- zlib-1.2.11-18.el8\_5.x86\_64
- redhat-lsb-core-4.1-47.el8.x86\_64 \*
- shadow-utils-4.6-16.el8.x86\_64 \*
- libstdc++-4.8.5-39.el7.x86\_64
- libuuid-2.23.2-63.el7.x86\_64
- libX11-1.6.7-4.el7\_9.x86\_64
- libXau-1.0.8-2.1.el7.x86\_64
- libxcb-1.13-1.el7.x86\_64
- libXext-1.3.3-3.el7.x86\_64
- libXrender-0.9.10-1.el7.x86\_64
- nss-softokn-freebl-3.67.0-3.el7\_9.x86\_64
- pam-1.1.8-23.el7.x86\_64
- zlib-1.2.7-20.el7\_9.x86\_64
- redhat-lsb-core-4.1-27.el7.centos.1.x86\_64 \*
- shadow-utils-4.6-5.el7.x86\_64 \*

### CentOS Linux release 7.9.2009

- audit-libs-2.8.5-4.el7.x86\_64
- bzip2-libs-1.0.6-13.el7.x86\_64
- fontconfig-2.13.0-4.3.el7.x86\_64
- freetype-2.8-14.el7\_9.1.x86\_64
- glibc-2.17-317.el7.x86\_64
- keyutils-libs-1.5.8-3.el7.x86\_64
- krb5-libs-1.15.1-50.el7.x86\_64
- libcap-ng-0.7.5-4.el7.x86\_64
- libcom\_err-1.42.9-19.el7.x86\_64
- libgcc-4.8.5-44.el7.x86\_64
- libpng-1.5.13-8.el7.x86\_64
- libselinux-2.5-15.el7.x86\_64

- libstdc++-4.8.5-44.el7.x86\_64
- libuuid-2.23.2-65.el7.x86\_64
- libX11-1.6.7-4.el7\_9.x86\_64
- libXau-1.0.8-2.1.el7.x86\_64
- libxcb-1.13-1.el7.x86\_64
- libXext-1.3.3-3.el7.x86\_64
- libXrender-0.9.10-1.el7.x86\_64
- nss-softokn-freebl-3.67.0-3.el7\_9.x86\_64
- pam-1.1.8-23.el7.x86\_64
- zlib-1.2.7-20.el7\_9.x86\_64
- redhat-lsb-core-4.1-27.el7.centos.1.x86\_64 \*
- shadow-utils-4.6-5.el7.x86\_64 \*

### **Verifying CentOS and Red Hat Libraries**

To verify that the appropriate package is installed on CentOS or Red Hat, enter:

rpm -q <package name>

If a required package is missing, you can download and install it using the yum command:

yum install <package name>

# **Linux Server Cluster Requirements**

This section describes the requirements of the Materials Server *only* on Linux clusters.

#### **Supported Operating Systems**

#### **IMPORTANT!** Installation of Materials Studio on Windows clusters is not supported.

Only x86-64 server operating systems are supported.

Operating System	Versions	Notes
Red Hat Enterprise Linux	7.5, 7.6, 7.7, 7.8, 7.9 8.2, 8.3, 8.4, 8.5, 8.6	
CentOS	7.5, 7.6, 7.7, 7.8, 7.9	8.x versions are no longer supported.

Currently, only the Forcite, Mesocite, CASTEP, DMol<sup>3</sup>, DFTB+, GULP, MesoDyn, and ONETEP servers are supported for parallel execution on Linux clusters. All server codes are supported for serial operation on Linux clusters. It is recommended to use one of the supported queuing systems to utilize computational resources of a Linux cluster efficiently.

- We support the same homogeneous clusters as Intel MPI.
- We support heterogeneous clusters with queuing systems that are configured to submit jobs to homogeneous subsets of the cluster.
- Compute nodes must be set up to communicate with each other and the head node through rsh or ssh without a password (for MPI).
- A license file or license server must be installed on the head node, unless the compute nodes are configured so that they can access a license server elsewhere.

Component	Minimum Hardware	Recommended	
Processor	Intel Xeon E5-1620 or equivalent	Intel Xeon Silver 41XX series or equivalent	
RAM per core (at least two cores)	2 GB	8 GB	
Available hard disk space for installation	4 GB	4 GB	
	Additional space is required if system updates are necessary.		
File system	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.		
Interconnects	Interconnect fabric supported by Intel MPI is required. See <u>https://software.intel.com/en-us/mpi-library</u> for more information.		

#### **Hardware Requirements**

Greater processing power and memory are recommended for any heavy duty use.

As you use Materials Studio to create structures, run calculations, gather and analyze results, the disk space required will increase to allow storage of both results and interim job files on the server. You should ensure that the server you use for Materials Studio has enough disk space to accommodate your long term space requirements.

It is *strongly* recommended that you use a <u>supported queuing system</u> to ensure an even distribution of jobs between the different processors. There are no graphics-related requirements for running Materials Studio on Linux clusters.

For details of Intel MPI, refer to the Intel Cluster MPI Libraries documentation (http://software.intel.com/en-us/articles/cluster-mpi-libraries/).

#### **Linux System Libraries**

On Linux systems, the standard C++ libraries for backward compatibility of the C++ compiler are required for proper operation of the Materials Studio server codes. These libraries should be installed prior to the installation of Materials Studio and BIOVIA License Pack. The packages that contain the required libraries are listed in the Linux Server System Libraries table.

## **Queuing Systems Requirements**

The following queuing systems are officially supported with the current version of Materials Studio:

Software	Versions	Operating Systems	Notes
Altair Portable Batch System (PBS) Pro	2020.x 2021.1 2022.1	Linux	https://www.altair.com/pbs- professional/
Slurm Workload Manager (SLURM)	20.11.x 21.08.x 22.0.5.x	Linux	https://slurm.schedmd.com

# **Finding Windows System Information**

Many system properties for computers running a Windows operating system are available from the System Properties page, which can be accessed from either the *Control Panel* or *Settings*.

More detailed information may be available from the following sources.

# Available Disk Space

In Windows File Explorer select the drive you want to check, right-click and select *Properties*. A pie chart shows how much free and used space is on the disk.

# **Operating System and Memory**

• Open Settings and choose System, then select About.

The operating system revision, including the service pack number, will be displayed in the panel on the right along with the amount of installed memory (RAM).

# **Microsoft Edge Version**

Start Microsoft Edge and access the Settings panel by clicking the ... and selecting *Settings*. The Microsoft Edge version information is displayed under the *About this app* heading.

## **Graphics Information**

To access the Windows graphics information:

• Open *Settings* and choose *System* then select *Display*. Click *Advanced display settings*.

The number of colors and desktop area are shown here.

#### Drivers

To access the graphics driver information:

• Click Advanced display settings then Display adapter properties.

This shows details of the graphics board on the Adapter tab.

Click the *Properties* button next to the details of the adapter. The driver version numbers can be accessed on the *Driver* tab.

# **Dassault Systèmes Support Resources**

For additional resources or to contact Dassault Systèmes Customer Support, visit the Support portal:

https://www.3ds.com/support/

From this portal, you can:

- Call or email Dassault Systèmes Customer Support
- Submit a request
- Download installers
- Access hardware and software requirements
- Access Knowledge Base
- Access Communities and Twitter feeds