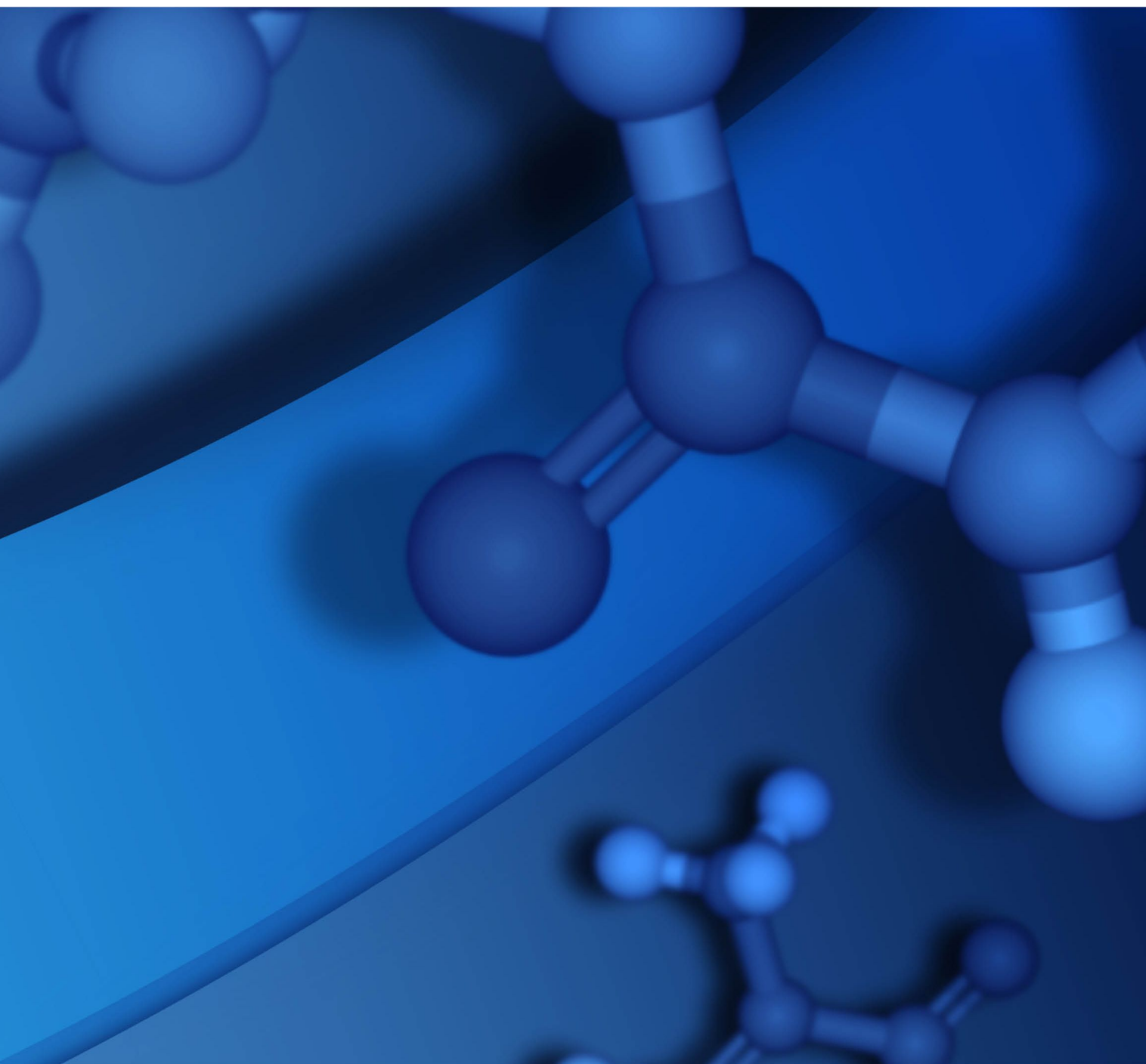


SYSTEM REQUIREMENTS

BIOVIA DISCOVERY STUDIO 2023 SP1



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Third Party Notification

Your BIOVIA Discovery Studio 2023 SP1 installation contains third-party software components. For details, refer to the BIOVIA Program Directory at <https://media.3ds.com/support/progdir/>.

Acknowledgments and References

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Chapter 1:

About This Document

This document describes the supported installation environments for BIOVIA Discovery Studio 2023 SP1.

Note: There are more specific requirements for users that want to run CHARMM OpenMM, ZDOCK, or NAMD jobs on a GPU in Discovery Studio. For more information, see [Operating Systems and CUDA Version for GPU Computing](#) on page 4.

Chapter 2:

Server Requirements

Operating Systems

Operating System	Versions	Comments
Microsoft® Windows Server	Windows Server 2019	64-bit only
	Windows Server 2016	64-bit only
Microsoft Windows	10	64-bit only standalone or single-user
CentOS	7.5+	64-bit only 8.x is not supported
Red Hat® Enterprise Linux®	8.2+	64-bit only
	7.9+	64-bit only

Hardware

Component	Minimum Hardware
Processor	Intel-compatible x86_64 architecture
RAM	4 GB per core 16 GB for a single core processor Note: Additional memory will increase performance.

Note: Protocols and Components with Python dependencies require CPUs with Advanced Vector Extensions (AVX) instructions.

Disk Space

The following table gives approximate space requirements for Discovery Studio.

Component	Approximate Size
Pipeline Pilot Server with Discovery Studio Collection	70 to 80 GB: 10 GB for Discovery Studio Collection. 10 to 20 GB for Pipeline Pilot Server components. 50 GB (minimum) of free disk space for runtime environment, user data files, etc.

Required BIOVIA Software

Software	Supported Versions	Notes
Pipeline Pilot Server	2023 SP1	BIOVIA Discovery Studio requires an installation of Pipeline Pilot Server. Refer to the <i>Discovery Studio Installation Guide</i> for details.
Pipeline Pilot Biology Collections third-party tools	2023 SP1	BIOVIA Discovery Studio relies on the Pipeline Pilot Sequence Analysis collection, which requires the separate installation of third-party tools that support the Pipeline Pilot Biology Collections. Refer to the <i>Discovery Studio Installation Guide</i> for details.

Supported BIOVIA Software

You can configure the Pipeline Pilot Server you are using with Discovery Studio to work with the following BIOVIA products.

Software	Supported Versions
BIOVIA Foundation Hub	2023 SP1

Additional Server Requirements

Supported Software for the Grid

Software	Version	Notes
PBS Pro	19.2	Linux only. https://www.altair.com/pbs-professional
Slurm Workload Manager (SLURM)	18.08.7 or later	Linux only. https://slurm.schedmd.com

Operating Systems and CUDA Version for GPU Computing

Note: See [Operating Systems](#) on page 2 for supported versions.

Executable	Protocols	Operating System	CUDA Version
CHARMM	▪ Dynamics (Production) ▪ MSLD Bias Optimization and Production ▪ CHARMM Relative FEP Calculations (GPU)	▪ Red Hat ▪ CentOS	10
ZDOCK	▪ Dock Protein (ZDOCK)	▪ Windows ▪ Red Hat ▪ CentOS	10
NAMD	▪ Dynamics (NAMD) ▪ Solvate with Explicit Membrane ▪ GaMD Production ▪ GaMD Equilibration	▪ Windows ▪ Red Hat ▪ CentOS	9

Notes:

- All the required CUDA libraries are included in the Discovery Studio server installation.
- CHARMM OpenMM (version 7.4) supports CUDA 10 and OpenCL 1.0.0 libraries. CHARMM DOMDEC supports CUDA 10, but not OpenCL
- For information about supported graphics cards for CUDA 9 and 10, see <https://en.wikipedia.org/wiki/CUDA>. NAMD supports Turing cards with special compilation options even though it is built with CUDA 9. Discovery Studio is certified on the following Turing cards: Quadro RTX 6000 and Tesla T4 listed in the table below.

Graphics Cards and Drivers for GPU Computing

The following combinations of NVIDIA graphics card, driver, and operating system are tested and certified:

Graphics Card	Driver Version	Operating System	Graphics Memory	Notes
GeForce GTX 1080 Ti	NVIDIA 440.44	Red Hat 7.9	11 GB	
Tesla T4	NVIDIA 470.57	CentOS 7.9	15 GB	
Quadro P5000	NVIDIA 470.57	Red Hat 7.9	16 GB	
Quadro RTX 6000	NVIDIA 450.66	Red Hat 8.2	24 GB	
Quadro K2200	NVIDIA 472.12	Windows Server 2019	4 GB	Not applicable to CHARMM

System Libraries (Linux Server)

Certain system libraries may be required for the Discovery Studio server on Red Hat and CentOS operating systems. The Discovery Studio distribution includes `check_system.sh`, which you can use to check which libraries may be required for your system.

Note: The libraries must be the 64-bit version.

- alsa-lib
- audit-libs
- bc
- bzip2-libs
- cairo
- compat-libstdc++-33
- compat-libtiff3
- e2fsprogs-libs
- expat
- fontconfig
- freetype
- gd
- glib2
- glibc
- keyutils-libs
- krb5-libs
- libdrm
- libgcc
- libICE
- libjpeg-turbo
- libnsl
- libpcap
- libpng15
- libsdl
- libsepol
- libSM
- libstdc++
- libX11
- libXau
- libXdamage
- libXdmcpr
- libXext
- libXfixes
- libXi
- libXinerama
- libXmu
- libXpm
- libXrender
- libXt
- libXtst
- libXxf86vm
- pam
- tcsh
- zlib

Chapter 3: Client Requirements

Operating Systems

Operating System	Versions	Notes
Microsoft Windows	11 Professional and Enterprise	64-bit only
	10 Professional and Enterprise	64-bit only
Red Hat Enterprise Linux	8.2+	64-bit only
	7.9+	64-bit only

Disk Space

Component	Approximate Size
Discovery Studio Client	1 GB

Graphics Cards

The Discovery Studio Client is supported on mid- to high-end graphic cards.

Browsers

IMPORTANT! A web browser is required to access Discovery Studio help.

Application	Versions	Notes
Mozilla Firefox	Latest ESR (Extended Support Release)	64-bit 32-bit compatible
Google Chrome	Latest version	64-bit
Microsoft Edge (Chromium version)	Latest version	64-bit

Note: To view the PDF format documentation included in the Discovery Studio help, you must have a PDF viewer installed on your machine. For Microsoft Edge you must have Adobe Reader installed, visit <https://get.adobe.com/uk/reader/>.

GNOME Desktop (Linux)

The Discovery Studio Client is optimized for the GNOME Desktop. You should install and configure this software, which is available on your Linux distribution media.

Note: KDE Desktop is also supported.

The Linux Discovery Studio Client requires certain system libraries which may not be installed by default. In such cases, the Discovery Studio Client may fail to launch and you will need to install the missing library.

Notes:

- libGLU and mesa-libGLU libraries are required for the Discovery Studio Client. Those libraries are part of the Window Manager installation (such as: Gnome or KDE).
- Red Hat 8 requires the installation of the libpng15 library for the Discovery Studio Client.

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 the Knowledge Base
- Access Communities and Twitter feeds