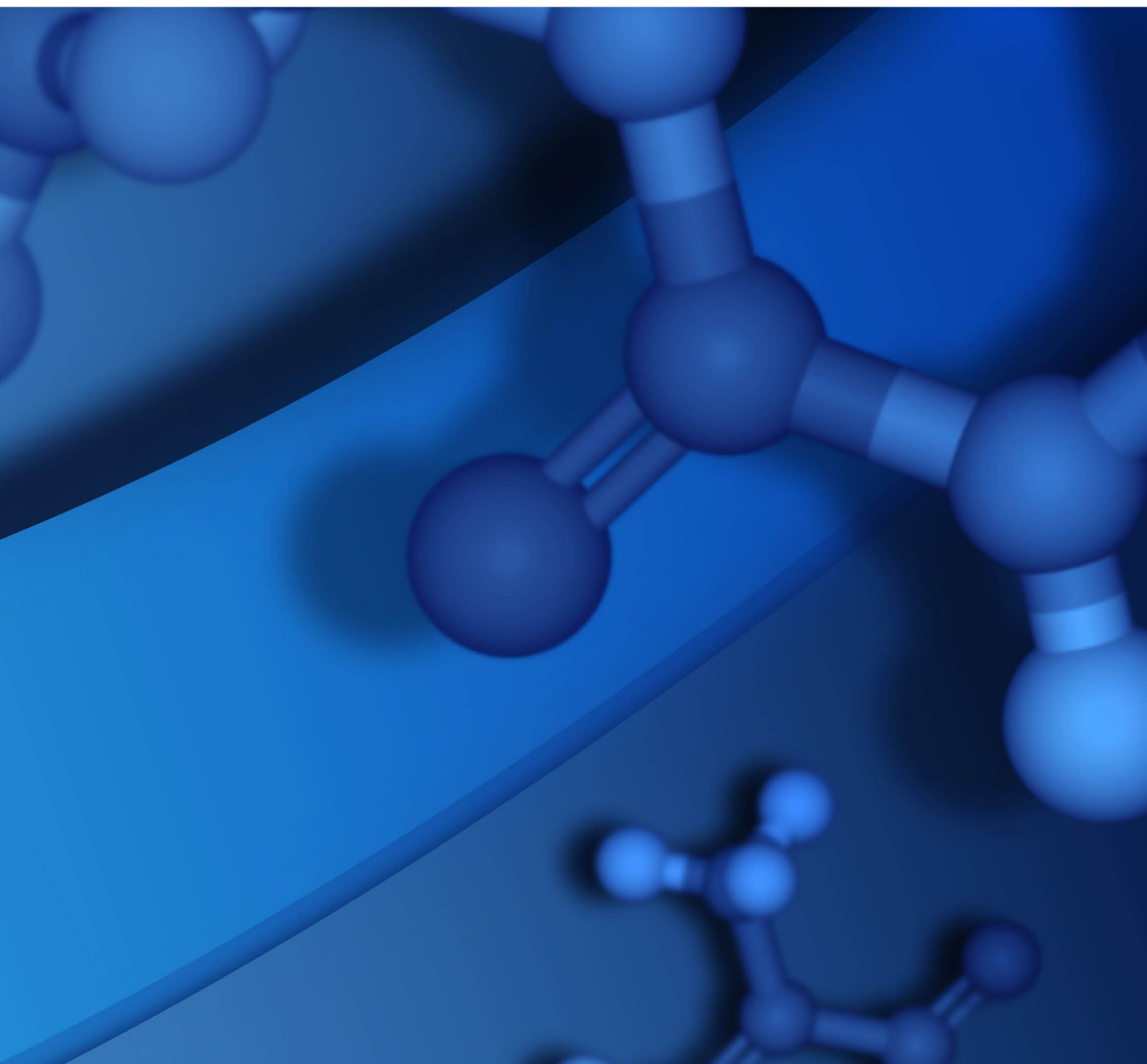


SYSTEM REQUIREMENTS

BIOVIA DISCOVERY STUDIO 2021



Copyright Notice

©2020 Dassault Systèmes. All rights reserved. 3DEXPERIENCE, the Compass icon and the 3DS logo, CATIA, SOLIDWORKS, ENOVIA, DELMIA, SIMULIA, GEOVIA, EXALEAD, 3DVIA, 3DSWYM, BIOVIA, NETVIBES, IFWE and 3DEXCITE, are commercial trademarks or registered trademarks of Dassault Systèmes, a French "société européenne" (Versailles Commercial Register # B 322 306 440), or its subsidiaries in the U.S. and/or other countries. All other trademarks are owned by their respective owners. Use of any Dassault Systèmes or its subsidiaries trademarks is subject to their express written approval.

Acknowledgments and References

To print photographs or files of computational results (figures and/or data) obtained by using Dassault Systèmes software, acknowledge the source in an appropriate format. For example:

"Computational results were obtained by using Dassault Systèmes BIOVIA software programs. BIOVIA Discovery Studio was used to perform the calculations and to generate the graphical results."

Dassault Systèmes may grant permission to republish or reprint its copyrighted materials. Requests should be submitted to Dassault Systèmes Customer Support, either by visiting <https://www.3ds.com/support/> and clicking **Call us** or **Submit a request**, or by writing to:

Dassault Systèmes Customer Support
10, Rue Marcel Dassault
78140 Vélizy-Villacoublay
FRANCE

Contents

About This Document	1
Definitions	1
System Requirements	2
Hardware Requirements	2
Disk Space	2
Graphics Cards	2
Supported Operating Systems	2
Server	2
Client	3
Supported Software for the Grid	3
GPU Requirements	3
Operating Systems and CUDA Version	3
Graphics Cards and Drivers for GPU Computing	4
BIOVIA Software	4
Required	4
Supported	4
Supported Browsers	4
Additional Requirements	5
GNOME Desktop (Linux)	5
System Libraries (Linux Server)	5
Dassault Systèmes Support Resources	7

About This Document

This document describes the supported installation environments for BIOVIA Discovery Studio 2021.

Note: There are more specific requirements for users who plan to run CHARMM OpenMM GPU in Discovery Studio. See [CHARMM OpenMM or DOMDEC GPU Requirements](#).

Definitions

The following defines specific terms for BIOVIA Discovery Studio 2021:

- **Supported:** The hardware or software was tested against BIOVIA Discovery 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 per 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 Discovery Studio.
- **Known to Be Incompatible:** Software, or versions of software, that will not function correctly in conjunction with BIOVIA Discovery Studio 2021.

System Requirements

Hardware Requirements

Component	Minimum Hardware
Processor	Intel-compatible x86_64 architecture
RAM	<ul style="list-style-type: none">■ 4 GB per core■ 16 GB for a single core processor <div style="border: 1px solid #ccc; padding: 5px; margin-top: 5px;">Note: Additional memory will increase performance.</div>

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. The databases listed below are optional but provide additional capabilities if they are installed.

Component	Approximate Size
Discovery Studio Client	1 GB
Discovery Studio server with Discovery Studio collections	25 GB

Graphics Cards

The Discovery Studio Client is supported on mid to high end graphic cards such as NVIDIA Quadro, AMD FirePro or Radeon.

Supported Operating Systems

Server

Operating System	Versions	Comments
Microsoft® Windows Server	Windows Server 2019	64-bit only
	Windows Server 2016	64-bit only
Microsoft Windows	10	64-bit standalone or single-user
CentOS	8.1+	64-bit only
	7.5+	64-bit only
Red Hat® Enterprise Linux®	8.1+	64-bit only
	7.5+	64-bit only

Client

Operating System	Versions	Notes
Windows	Windows 10	64-bit
Red Hat Enterprise Linux	8.1+	64-bit
	7.5+	64-bit

Supported Software for the Grid

Software	Version
PBS	18.2.3
Slurm	18.08

GPU Requirements

Operating Systems and CUDA Version

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

Executable	Protocols	Operating System	CUDA Version
CHARMm	<ul style="list-style-type: none"> ■ Dynamics (Production) ■ MSLD Bias Optimization and Production ■ CHARMm Relative FEP Calculations (GPU) 	<ul style="list-style-type: none"> ■ Red Hat ■ CentOS 	10
ZDOCK	<ul style="list-style-type: none"> ■ Dock Protein (ZDOCK) 	<ul style="list-style-type: none"> ■ Windows ■ Red Hat ■ CentOS 	10
NAMD	<ul style="list-style-type: none"> ■ Dynamics (NAMD) ■ Solvate with Explicit Membrane 	<ul style="list-style-type: none"> ■ 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 7.8	11 GB	
Tesla T4	NVIDIA 440.64	CentOS 7.8	15 GB	
Quadro GP100	NVIDIA 440.100	CentOS 8.2	16 GB	
Quadro P5000	NVIDIA 440.64	Red Hat 7.8	16 GB	
Quatro RTX 6000	NVIDIA 450.66	Red Hat 8.2	24 GB	
Quadro K2200	NVIDIA 431.70	Windows Server 2019	4 GB	Not applicable to CHARMM

BIOVIA Software

Required

Software	Supported Versions	Notes
Pipeline Pilot Biology Collections third-party tools	2021	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 about installing them.

Supported

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	2021

Supported Browsers

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

Application	Versions	Notes
Microsoft Internet Explorer	11	
Microsoft Edge	Latest	At the time of release this is 44
Google Chrome	Latest	At the time of release this is 85
Mozilla Firefox	78.3.0 ESR	

Note: In order 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 and Internet Explorer 11 you must have Adobe Reader installed, visit <https://get.adobe.com/uk/reader/>.

Additional Requirements

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 and CentOS 8 require the installation of the libpng15 library for the Discovery Studio Client.

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 that the libraries must be the 64-bit version.

- | | | |
|-----------------------|-----------------|---------------|
| ■ alsa-lib | ■ keyutils-libs | ■ libXdmcp |
| ■ audit-libs | ■ krb5-libs | ■ llibXext |
| ■ bc | ■ libdrm | ■ libXfixes |
| ■ bzip2-libs | ■ libgcc | ■ libXi |
| ■ cairo | ■ libICE | ■ libXinerama |
| ■ compat-libstdc++-33 | ■ libjpeg-turbo | ■ libXmu |
| ■ compat-libtiff3 | ■ libnsl | ■ libXpm |
| ■ e2fsprogs-libs | ■ libpcap | ■ libXrender |

System Requirements

- expat
- fontconfig
- freetype
- gd
- glib2
- glibc
- libpng15
- libselinux
- libsepol
- libSM
- libstdc++
- libX11
- libXau
- libXdamage
- libXt
- libXtst
- libXxf86vm
- pam
- tcsh
- zlib

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