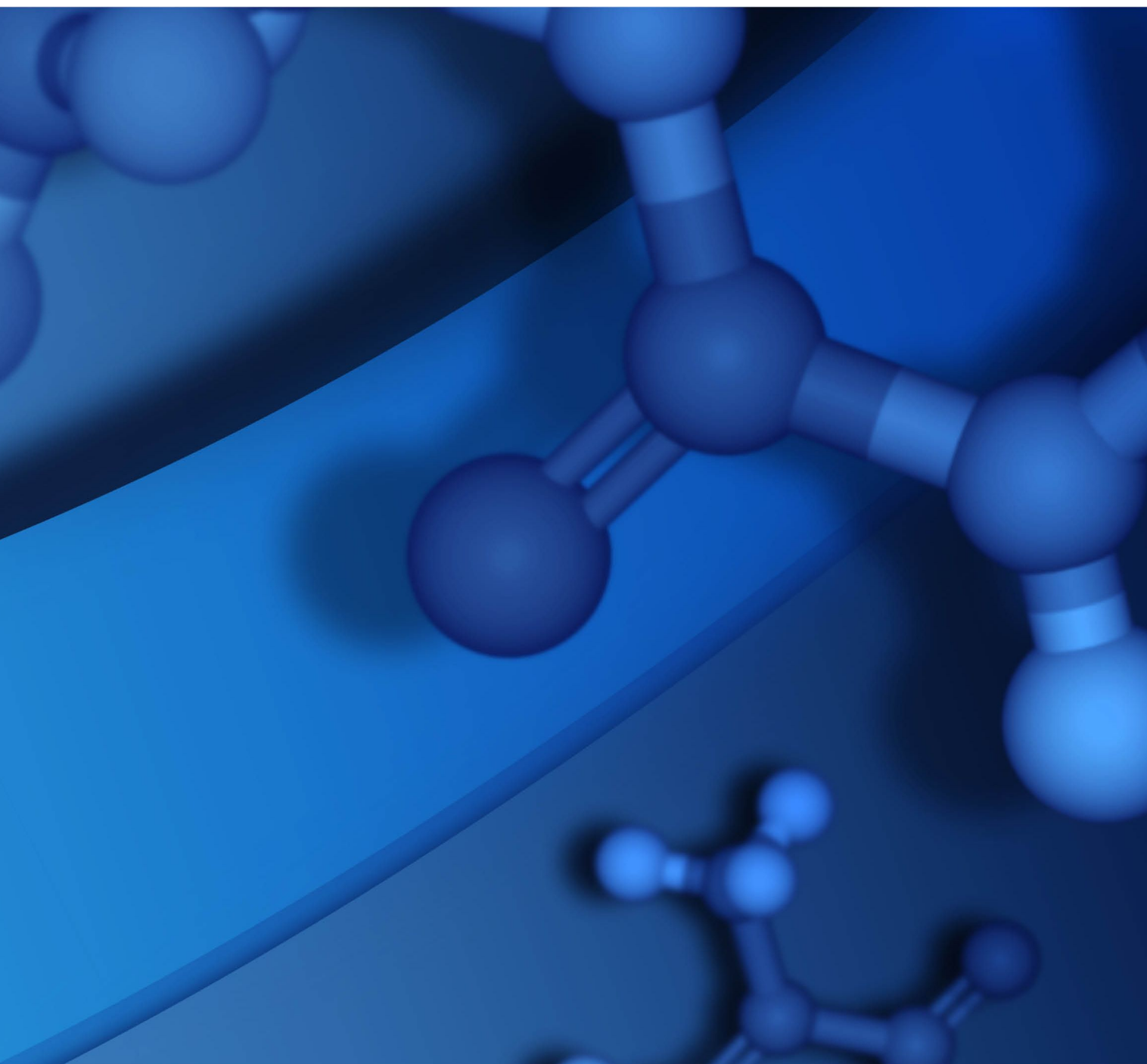


# SYSTEM REQUIREMENTS

BIOVIA DISCOVERY STUDIO 2022



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## Acknowledgments and References

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## About This Document

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This document describes the supported installation environments for BIOVIA Discovery Studio 2022.

**Note:** There are more specific requirements for users planning to running CHARMM OpenMM, ZDOCK, or NAMD jobs on a GPU in Discovery Studio. For more information, see [GPU Requirements](#) on page 3.

## Definitions

The following defines specific terms for BIOVIA Discovery Studio 2022:

- **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 2022.

# System Requirements

## Hardware Requirements

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

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
	Windows Server 2016	64-bit
Microsoft Windows	10	64-bit standalone or single-user
CentOS	7.5+	64-bit 8.x versions are no longer supported.
Red Hat® Enterprise Linux®	8.1+	64-bit
	7.5+	64-bit

## Client

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

## Supported Software for the Grid

Software	Version	Notes
Altair Portable Batch System (PBS) Pro	19.2	Linux only. <a href="https://www.altair.com/pbs-professional/">https://www.altair.com/pbs-professional/</a>
Slurm Workload Manager (SLURM)		Linux only. <a href="https://slurm.schedmd.com">https://slurm.schedmd.com</a>

## 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"> <li>▪ Dynamics (Production)</li> <li>▪ MSLD Bias Optimization and Production</li> <li>▪ CHARMm Relative FEP Calculations (GPU)</li> </ul>	<ul style="list-style-type: none"> <li>▪ Red Hat</li> <li>▪ CentOS</li> </ul>	10
ZDOCK	<ul style="list-style-type: none"> <li>▪ Dock Protein (ZDOCK)</li> </ul>	<ul style="list-style-type: none"> <li>▪ Windows</li> <li>▪ Red Hat</li> <li>▪ CentOS</li> </ul>	10
NAMD	<ul style="list-style-type: none"> <li>▪ Dynamics (NAMD)</li> <li>▪ Solvate with Explicit Membrane</li> </ul>	<ul style="list-style-type: none"> <li>▪ Windows</li> <li>▪ Red Hat</li> <li>▪ CentOS</li> </ul>	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	
Quatro 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

## BIOVIA Software

### Required

Software	Supported Versions	Notes
Pipeline Pilot Biology Collections third-party tools	2022	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	2022



## Supported Browsers

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

Application	Versions	Notes
Microsoft Edge (Chromium) 64-bit	Latest	At the time of release this is 93
Google Chrome 64-bit	Latest	At the time of release this is 93
Mozilla Firefox 64-bit and 42-bit compatible	78 ESR or later	

**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 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 requires 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:** The libraries must be the 64-bit version.

- |                       |                 |               |
|-----------------------|-----------------|---------------|
| ▪ alsa-lib            | ▪ keyutils-libs | ▪ libXdmcpc   |
| ▪ 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

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

## Dassault Systèmes Support Resources

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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