Local Installation

Introduction

This guide walks through how to install CUDA Quantum on your system, and how to set up VS Code for local development. The section on connecting to a remote host contains some guidance for application development on a remote host where CUDA Quantum is installed.

The following sections contain instructions for how to install CUDA Quantum on your machine using

- Docker: A fully featured CUDA Quantum installation including all C++ and Python tools is available as a Docker image.
- Singularity: A Singularity container can easily be created based on our Docker images.
- PyPI: Additionally, we distribute pre-built Python wheels via PyPI.
- Pre-built binaries: We also provide pre-built C++ binaries, bundled as self-extracting archive, that work across a range of Linux operating systems.

If you would like to build CUDA Quantum from source to deploy on an HPC system without relying on a container runtime, please follow the instructions for Installation from Source. If, on the other hand, you want to contribute to the development of CUDA Quantum itself and hence want to build a custom version of CUDA Quantum from source, follow the instructions on the CUDA Quantum GitHub repository instead.

If you are unsure which option suits you best, we recommend using our Docker image to develop your applications in a controlled environment that does not depend on, or interfere with, other software that is installed on your system.

Docker

To download and use our Docker images, you will need to install and launch the Docker engine. If you do not already have Docker installed on your system, you can get it by downloading and installing Docker Desktop. If you do not have the necessary administrator permissions to install software on your machine, take a look at the section below on how to use Singularity instead.

Docker images for all CUDA Quantum releases are available on the NGC Container Registry. In addition to publishing stable releases, we also publish Docker images whenever we update certain branches on our GitHub repository. These images are published in our nightly channel on NGC. To download the latest version on the main branch of our GitHub repository, for example, use the command

```
docker pull nvcr.io/nvidia/nightly/cuda-quantum:latest
```

Early prototypes for features we are considering can be tried out by using the image tags starting with `experimental`. The `README` in the `/home/cudaq` folder in the container gives more details about the feature. We welcome and appreciate your feedback about these early prototypes; how popular they are will help inform whether we should include them in future releases.

Once you have downloaded an image, the container can be run using the command

```
docker run -it --name cuda-quantum nvcr.io/nvidia/nightly/cuda-quantum:latest
```

Replace the image name and/or tag in the command above, if necessary, with the one you want to use. This will give you terminal access to the created container. To enable support for GPU-accelerated backends, you will need to pass the `--gpus` flag when launching the container, for example:

```
docker run -it --gpus all --name cuda-quantum nvcr.io/nvidia/nightly/cuda-quantum:latest
```

Note

This command will fail if you do not have a suitable NVIDIA GPU available, or if your driver version is insufficient. To improve compatibility with older drivers, you may need to install the NVIDIA container toolkit.

You can stop and exit the container by typing the command `exit`. If you did not specify `--rm` flag when launching the container, the container still exists after exiting, as well as any changes you made in it. You can get back to it using the command `docker start -i cuda-quantum`. You can delete an existing container and any changes you made using `docker rm -v cuda-quantum`.

When working with Docker images, the files inside the container are not visible outside the container environment. To facilitate application development with, for example, debugging, code completion, hover information, and so on, please take a look at the section on Development with VS Code.

Alternatively, it is possible, but not recommended, to launch an SSH server inside the container environment and connect an IDE using SSH. To do so, make sure you have generated a suitable RSA key pair; if your `~/.ssh/` folder does not already contain the files `id_rsa.pub` and `id.rsa`, follow the instructions for generating a new SSH key on this page. You can then launch the container and connect to it via SSH by executing the following commands:

```
docker run -itd --gpus all --name cuda-quantum -p 2222:22 nvcr.io/nvidia/nightly/cuda-quantum:latest
docker exec cuda-quantum bash -c "sudo apt-get install -y --no-install-recommends openssh-server"
docker exec cuda-quantum bash -c "sudo sed -i -E "s/#?\s*UsePAM\s+.+/UsePAM yes/g" /etc/ssh/sshd_config"
docker cp ~/.ssh/id_rsa.pub cuda-quantum:/home/cudaq/.ssh/authorized_keys
docker exec -d cuda-quantum bash -c "sudo -E /usr/sbin/sshd -D"
ssh cudaq@localhost -p 2222 -o StrictHostKeyChecking=no -o UserKnownHostsFile=/dev/null -o GlobalKnownHostsFile=/dev/null
```

Singularity

You can use Singularity to run a CUDA Quantum container in a folder without needing administrator permissions. If you do not already have Singularity installed, you can build a relocatable installation from source. To do so on Linux or WSL, make sure you have the necessary prerequisites installed, download a suitable version of the go toolchain, and make sure the `go` binaries are on your `PATH`. You can then build Singularity with the commands

```
wget https://github.com/sylabs/singularity/releases/download/v4.0.1/singularity-ce-4.0.1.tar.gz
tar -xzf singularity-ce-4.0.1.tar.gz singularity-ce-4.0.1/ && rm singularity-ce-4.0.1.tar.gz && cd singularity-ce-4.0.1/
./mconfig --without-suid --prefix="$HOME/.local/singularity"
make -C ./builddir && make -C ./builddir install && cd .. && rm -rf singularity-ce-4.0.1/
echo 'PATH="$PATH:$HOME/.local/singularity/bin/"' >> ~/.profile && source ~/.profile
```

For more information about using Singularity on other systems, take a look at the admin guide.

Once you have singularity installed, create a file `cuda-quantum.def` with the following content:

```
Bootstrap: docker
From: nvcr.io/nvidia/nightly/cuda-quantum:latest

%runscript
    mount devpts /dev/pts -t devpts
    cp -r /home/cudaq/* .
    bash
```

Replace the image name and/or tag in the `From` line, if necessary, with the one you want to use; In addition to publishing stable releases, we also publish Docker images whenever we update certain branches on our GitHub repository. These images are published in our nightly channel on NGC. Early prototypes for features we are considering can be tried out by using the image tags starting with `experimental`. We welcome and appreciate your feedback about these early prototypes; how popular they are will help inform whether we should include them in future releases.

You can then create a CUDA Quantum container by running the following commands:

```
singularity build --fakeroot cuda-quantum.sif cuda-quantum.def
singularity run --writable --fakeroot cuda-quantum.sif
```

In addition to the files in your current folder, you should now see a `README` file, as well as examples and tutorials. To enable support for GPU-accelerated backends, you will need to pass the the `--nv` flag when running the container:

```
singularity run --writable --fakeroot --nv cuda-quantum.sif
nvidia-smi
```

The output of the command above lists the GPUs that are visible and accessible in the container environment.

Note

If you do not see any GPUs listed in the output of `nvidia-smi`, it means the container environment is unable to access a suitable NVIDIA GPU. This can happen if your driver version is insufficient, or if you are working on WSL. To improve compatibility with older drivers, or to enable GPU support on WSL, please install the NVIDIA container toolkit, and update the singularity configuration to set `use nvidia-container-cli` to `yes` and configure the correct `nvidia-container-cli path`. The two commands below use `sed` to do that:

```
sed -i 's/use nvidia-container-cli = no/use nvidia-container-cli = yes/'
"$HOME/.local/singularity/etc/singularity/singularity.conf"
sed -i 's/# nvidia-container-cli path =/nvidia-container-cli path =
\/usr\/bin\/nvidia-container-cli/'
"$HOME/.local/singularity/etc/singularity/singularity.conf"
```

You can exit the container environment by typing the command `exit`. Any changes you made will still be visible after you exit the container, and you can re-enable the container environment at any time using the `run` command above.

To facilitate application development with, for example, debugging, code completion, hover information, and so on, please take a look at the section on Development with VS Code.

Python wheels

CUDA Quantum Python wheels are available on PyPI.org. Installation instructions can be found in the project description. For more information about available versions and documentation, see CUDA Quantum Releases.

There are currently no source distributions available on PyPI, but you can download the source code for the latest version of the CUDA Quantum Python wheels from our GitHub repository. The source code for previous versions can be downloaded from the respective GitHub Release.

At this time, wheels are distributed for Linux operating systems only. If your platform is not officially supported and `pip` does not find a compatible wheel to install, you can build your own wheel from source following the instructions here: Installation from Source.

To build the CUDA Quantum Python API for the purpose of contributing to our GitHub repository, follow the instructions for Setting up your Environment, and then run the following commands in the repository root:

```
bash scripts/install_prerequisites.sh
pip install . --user
```

Pre-built binaries

Starting with the 0.6.0 release, we provide pre-built binaries for using CUDA Quantum with C++. Support for using CUDA Quantum with Python can be installed side-by-side with the pre-built binaries for C++ by following the instructions on PyPI.org. The pre-built binaries work across a range of Linux operating systems listed under Dependencies and Compatibility.

Before installing our pre-built binaries, please make sure that your operating system is using the GNU C library version 2.28 or newer. You can confirm this by checking the output of the command `ldd --version`. If this command does not exist, or shows an older version than 2.28, please double check that your operating system is listed as supported. If you use an operating system with an older GNU C library version, you will need to build the installer from source following the instructions in Installation from Source.

You can download the `install_cuda_quantum` file for your processor architecture from the assets of the respective GitHub release. The installer is a self-extracting archive that contains the pre-built binaries as well as a script to move them to the correct locations. You will need `bash`, `tar`, and `gzip` (usually already installed on most Linux distributions) to run the installer. The installation location of CUDA Quantum is not currently configurable and using the installer hence requires admin privileges on the system. We may revise that in the future; please see and upvote the corresponding GitHub issue.

To install CUDA Quantum, execute the command

```
MPI_PATH=/usr/local/openmpi \
sudo -E bash install_cuda_quantum.$(uname -m) --accept && . /etc/profile
```

Note

To use GPU-accelerated backends, you will need to install the necessary CUDA runtime libraries. For more information see the corresponding section on Additional CUDA Tools.

The installation ensures that the necessary environment variables for using the CUDA Quantum toolchain are set upon login for all POSIX shells. Confirm that the `nvq++` command is found. If it is not, please make sure to set the environment variables defined by the `set_env.sh` script in the CUDA Quantum installation folder (usually `/opt/nvidia/cudaq`).

If an MPI installation is available in the directory defined by `MPI_PATH`, the installer automatically enables MPI support in CUDA Quantum. If you do not have MPI installed on your system, you can simply leave that path empty, and CUDA Quantum will be installed without MPI support. If you install MPI at a later point in time, you can activate the MPI support in CUDA Quantum by setting the `MPI_PATH` variable to its installation location and executing the commands

```
MPI_PATH=/usr/local/openmpi # update this path as needed
bash "${CUDA_QUANTUM_PATH}/distributed_interfaces/activate_custom_mpi.sh"
```

To develop C++ code, you most likely also want to install the C++ standard library. CUDA Quantum supports the GNU C++ standard library (`libstdc++`), version 11 or newer. Other libraries may work but can cause issues in certain cases. The C++ standard library, including development headers, is almost certainly available via the package manager for your system. To ensure the libraries and headers are discoverable, the easiest option is usually to install the complete GCC toolchain. Note that for certain distributions, you may need to manually enable that version after installation by running a script called `enable`. You can search for such a script with the command `find / -path '*gcc*' -name enable`.

Development with VS Code

To facilitate application development with, for example, debugging, code completion, hover information, and so on, we recommend using VS Code. VS Code provides a seamless development experience on all platforms, and is also available without installation via web browser. This sections describes how to connect VS Code to a running container on your machine. The section on connecting to a remote host contains information on how to set up your development environment when accessing CUDA Quantum on a remote host instead.

Using a Docker container

Before connecting VS Code, open a terminal/shell, and start the CUDA Quantum Docker container following the instructions in the section above.

If you have a local installation of VS Code you can connect to the running container using the Dev Containers extension. If you want to use VS Code in the web browser, please follow the instructions in the section Developing with Remote Tunnels instead.

After installing the Dev Containers extension, launch VS Code, open the Command Palette with `Ctrl+Shift+P`, and enter "Dev Containers: Attach to Running Container". You should see and select the running `cuda-quantum` container in the list. After the window reloaded, enter "File: Open Folder" in the Command Palette to open the `/home/cudaq/` folder.

To run the examples, open the Command Palette and enter "View: Show Terminal" to launch an integrated terminal. You are now all set to get started with CUDA Quantum development.

Using a Singularity container

If you have a GitHub or Microsoft account, we recommend that you connect to a CUDA Quantum container using tunnels. To do so, launch a CUDA Quantum Singularity container following the instructions in the section above, and then follow the instructions in the section Developing with Remote Tunnels.

If you cannot use tunnels, you need a local installation of VS Code and you need to install the Remote - SSH extension. Make sure you also have a suitable SSH key pair; if your `~/.ssh/` folder does not already contain the files `id_rsa.pub` and `id.rsa`, follow the instructions for generating a new SSH key on this page.

To connect VS Code to a running CUDA Quantum container, the most convenient setup is to install and run an SSH server in the Singularity container. Open a terminal/shell in a separate window, and enter the following commands to create a suitable sandbox:

```
singularity build --sandbox cuda-quantum-sandbox cuda-quantum.sif
singularity exec --writable --fakeroot cuda-quantum-sandbox \
  apt-get install -y --no-install-recommends openssh-server
cat ~/.ssh/id_rsa.pub >> ~/.ssh/authorized_keys
```

You can launch this sandbox by entering the commands below. Please see the Singularity section above for more information about how to get the `cuda-quantum.sif` image, and how to enable GPU-acceleration with the `--nv` flag.

```
singularity run --writable --fakeroot --nv --network-args="portmap=22:2222/tcp" cuda-
quantum-sandbox
/usr/sbin/sshd -D -p 2222 -E sshd_output.txt
```

> **Note**
>
> Make sure to use a free port. You can check if the SSH server is ready and listening by looking at the log in `sshd_output.txt`. If the port is already in use, you can replace the number `2222` by any free TCP port in the range `1025-65535` in all commands.

Entering `Ctrl+C` followed by `exit` will stop the running container. You can re-start it at any time by entering the two commands above. While the container is running, open the Command Palette in VS Code with `Ctrl+Shift+P`, enter “Remote-SSH: Add new SSH Host”, and enter the following SSH command:

```
ssh root@localhost -p 2222 -o StrictHostKeyChecking=no -o UserKnownHostsFile=/dev/null -o
GlobalKnownHostsFile=/dev/null
```

> **Note**

> If you are working on Windows and are building and running the Singularity container in WSL, make sure to copy the used SSH keys to the Windows partition, such that VS Code can connect with the expected key. Alternatively, add the used public key to the `/root/.ssh/authorized_keys` file in the Singularity container.

You can then connect to the host by opening the Command Palette, entering "Remote SSH: Connect Current Window to Host", and choosing the newly created host. After the window reloaded, enter "File: Open Folder" in the Command Palette to open the desired folder.

To run the examples, open the Command Palette and enter "View: Show Terminal" to launch an integrated terminal. You are now all set to get started with CUDA Quantum development.

Connecting to a Remote Host

Depending on the setup on the remote host, there are a couple of different options for developing CUDA Quantum applications.

- If a CUDA Quantum container is running on the remote host, and you have a GitHub or Microsoft account, take a look at Developing with Remote Tunnels. This works for both Docker and Singularity containers on the remote host, and should also work for other containers.
- If you cannot use tunnels, or if you want to work with an existing CUDA Quantum installation without using a container, take a look at Remote Access via SSH instead.

Developing with Remote Tunnels

Remote access via tunnel can easily be enabled with the VS Code CLI. This allows to connect either a local installation of VS Code, or the VS Code Web UI, to a running CUDA Quantum container on the same or a different machine.

Creating a secure connection requires authenticating with the same GitHub or Microsoft account on each end. Once authenticated, an SSH connection over the tunnel provides end-to-end encryption. To download the VS Code CLI, if necessary, and create a tunnel, execute the following command in the running CUDA Quantum container, and follow the instructions to authenticate:

```
vscode-setup tunnel --name cuda-quantum-remote --accept-server-license-terms
```

You can then either open VS Code in a web browser, or connect a local installation of VS Code. To connect a local installation of VS Code, make sure you have the Remote - Tunnels extension installed, then open the Command Palette with `Ctrl+Shift+P`, enter “Remote Tunnels: Connect to Tunnel”, and enter `cuda-quantum-remote`. After the window reloaded, enter “File: Open Folder” in the Command Palette to open the `/home/cudaq/` folder.

You should see a pop up asking if you want to install the recommended extensions. Selecting to install them will configure VS Code with extensions for working with C++, Python, and Jupyter. You can always see the list of recommended extensions that aren’t installed yet by clicking on the “Extensions” icon in the sidebar and navigating to the “Recommended” tab.

Remote Access via SSH

To facilitate application development with, for example, debugging, code completion, hover information, and so on, you can connect a local installation of VS Code to a remote host via SSH.

> **Note**
>
> For the best user experience, we recommend to launch a CUDA Quantum container on the remote host, and then connect VS Code using tunnels. If a connection via tunnel is not possible, this section describes using SSH instead.

To do so, make sure you have Remote - SSH extension installed. Open the Command Palette with `Ctrl+Shift+P`, enter “Remote-SSH: Add new SSH Host”, and enter the SSH command to connect to your account on the remote host. You can then connect to the host by opening the Command Palette, entering “Remote SSH: Connect Current Window to Host”, and choosing the newly created host.

When prompted, choose Linux as the operating system, and enter your password. After the window reloaded, enter “File: Open Folder” in the Command Palette to open the desired folder. Our GitHub repository contains a folder with VS Code configurations including a list of recommended extensions for working with CUDA Quantum; you can copy these configurations into the a folder named `.vscode` in your workspace to use them.

If you want to work with an existing CUDA Quantum installation on the remote host, you are all set. Alternatively, you can use Singularity to build and run a container following the instructions in this section. Once the `cuda-quantum.sif` image is built and available in your home directory on the remote host, you can update your VS Code configuration to enable/improve completion, hover information, and other development tools within the container.

To do so, open the Command Palette and enter "Remote-SSH: Open SSH Configuration File". Add a new entry to that file with the command to launch the container, and edit the configuration of the remote host, titled `remote-host` in the snippets below, to add a new identifier:

```
Host cuda-quantum~*
  RemoteCommand singularity run --writable --fakeroot --nv ~/cuda-quantum.sif
  RequestTTY yes

Host remote-host cuda-quantum~remote-host
  HostName ...
  ...
```

You will need to edit a couple of VS Code setting to make use of the newly defined remote command; open the Command Palette, enter "Preferences: Open User Settings (JSON)", and add or update the following configurations:

```
"remote.SSH.enableRemoteCommand": true,
"remote.SSH.useLocalServer": true,
"remote.SSH.remoteServerListenOnSocket": false,
"remote.SSH.connectTimeout": 120,
"remote.SSH.serverInstallPath": {
    "cuda-quantum~remote-host": "~/.vscode-container/cuda-quantum",
},
```

After saving the changes, you should now be able to select `cuda-quantum~remote-host` as the host when connecting via SSH, which will launch the CUDA Quantum container and connect VS Code to it.

> **Note**
>
> If the connection to `cuda-quantum~remote-host` fails, you may need to specify the full path to the `singularity` executable on the remote host, since environment variables, and specifically the configured `PATH` may be different during launch than in your user account.

DGX Cloud

If you are using DGX Cloud, you can easily use it to run CUDA Quantum applications. While submitting jobs to DGX Cloud directly from within CUDA Quantum is not (yet) supported, you can use the NGC CLI to launch and interact with workloads in DGX Cloud. The following sections detail how to do that, and how to connect JupyterLab and/or VS Code to a running CUDA Quantum job in DGX Cloud.

Get Started

To get started with DGX Cloud, you can request access here. Once you have access, sign in to your account, and generate an API key. Install the NGC CLI and configure it with

```
ngc config set
```

entering the API key you just generated when prompted, and configure other settings as appropriate.

Note

The rest of this section assumes you have CLI version 3.33.0. If you have an older version installed, you can upgrade to the latest version using the command

```
ngc version upgrade 3.33.0
```

See also the NGC CLI documentation for more information about available commands.

You can see all information about available compute resources and ace instances with the command

```
ngc base-command ace list
```

Confirm that you can submit a job with the command

```
ngc base-command job run \
  --name Job-001 --total-runtime 60s \
  --image nvcr.io/nvidia/nightly/cuda-quantum:latest --result /results \
  --ace <ace_name> --instance <instance_name> \
  --commandline 'echo "Hello from DGX Cloud!"'
```

replacing `<ace_name>` and `<instance_name>` with the name of the ace and instance you want to execute the job on. You should now see that job listed when you run the command

```
ngc base-command job list
```

Once it has completed you can download the job results using the command

```
ngc base-command result download <job_id>
```

replacing `<job_id>` with the id of the job you just submitted. You should see a new folder named `<job_id>` with the job log that contains the output "Hello from DGX Cloud!".

For more information about how to use the NGC CLI to interact with DGX Cloud, we refer to the NGC CLI documentation.

Use JupyterLab

Once you can run jobs on DGX Cloud, you can launch an interactive job to use CUDA Quantum with JupyterLab running on DGX Cloud:

```
ngc base-command job run \
  --name Job-interactive-001 --total-runtime 600s \
  --image nvcr.io/nvidia/nightly/cuda-quantum:latest --result /results \
  --ace <ace_name> --instance <instance_name> \
  --port 8888 --commandline 'jupyter-lab-setup <my-custom-token> --port=8888'
```

Replace `<my-custom-token>` in the command above with a custom token that you can freely choose. You will use this token to authenticate with JupyterLab; Go to the job portal, click on the job you just launched, and click on the link under "URL/Hostname" in Service Mapped Ports.

> **Note**
>
> It may take a couple of minutes for DGX Cloud to launch and for the URL to become active, even after it appears in the Service Mapped Ports section; if you encounter a "404: Not Found" error, be patient and try again in a couple of minutes.

Once this URL opens, you should see the JupyterLab authentication page; enter the token you selected above to get access to the running CUDA Quantum container. On the left you should see a folder with tutorials. Happy coding!

Use VS Code

Once you can run jobs on DGX Cloud, you can launch an interactive job to use CUDA Quantum with a local installation of VS Code, or the VS Code Web UI, running on DGX Cloud:

```
ngc base-command job run \
  --name Job-interactive-001 --total-runtime 600s \
  --image nvcr.io/nvidia/nightly/cuda-quantum:latest --result /results \
  --ace <ace_name> --instance <instance_name> \
  --commandline 'vscode-setup tunnel --name cuda-quantum-dgx --accept-server-license-terms'
```

Go to the job portal, click on the job you just launched, and select the "Log" tab. Once the job is running, you should see instructions there for how to connect to the device the job is running on. These instructions include a link to open and the code to enter on that page; follow the instructions to authenticate. Once you have authenticated, you can either open VS Code in a web browser, or connect a local installation of VS Code. To connect a local installation of VS Code, make sure you have the Remote - Tunnels extension installed, then open the Command Palette with `Ctrl+Shift+P`, enter "Remote Tunnels: Connect to Tunnel", and enter `cuda-quantum-remote`. After the window reloaded, enter "File: Open Folder" in the Command Palette to open the `/home/cudaq/` folder.

You should see a pop up asking if you want to install the recommended extensions. Selecting to install them will configure VS Code with extensions for working with C++, Python, and Jupyter. You can always see the list of recommended extensions that aren't installed yet by clicking on the "Extensions" icon in the sidebar and navigating to the "Recommended" tab.

If you enter "View: Show Explorer" in the Command Palette, you should see a folder with tutorials and examples to help you get started. Take a look at Next Steps to dive into CUDA Quantum development.

Additional CUDA Tools

CUDA Quantum makes use of GPU-acceleration in certain backends and components. Depending on how you installed CUDA Quantum, you may need to install certain CUDA libraries separately to take advantage of these.

Installation via PyPI

If you installed CUDA Quantum via PyPI, please follow the installation instructions there to install the necessary CUDA dependencies.

Installation In Container Images

If you are using the CUDA Quantum container image, the image already contains all necessary runtime libraries to use all CUDA Quantum components. To take advantage of GPU-acceleration, make sure to enable GPU support when you launch the container, that is pass the

`--gpus all` flag when launching the container with Docker and the `--nv` flag when launching the container with Singularity.

Note that the image does not contain all development dependencies for CUDA, such as, for example the `nvcc` compiler. You can install all CUDA development dependencies by running the command

```
sudo apt-get install cuda-toolkit-11.8
```

inside the container. Most Python packages that use GPU-acceleration, such as for example CuPy, require an existing CUDA installation. After installing the `cuda-toolkit-11.8` you can install CuPy with the command

```
python3 -m pip install cupy-cuda11x
```

Installing Pre-built Binaries

If you installed pre-built binaries for CUDA Quantum, you will need to install the necessary CUDA runtime libraries to use GPU-acceleration in CUDA Quantum. If you prefer to only install the minimal set of runtime libraries, the following commands, for example, install the necessary packages for RHEL 8:

```
CUDA_VERSION=11.8
CUDA_DOWNLOAD_URL=https://developer.download.nvidia.com/compute/cuda/repos
# Go to the url above, set the variables below to a suitable distribution
# and subfolder for your platform, and uncomment the line below.
# DISTRIBUTION=rhel8 CUDA_ARCH_FOLDER=x86_64

version_suffix=$(echo ${CUDA_VERSION} | tr . -)
dnf config-manager --add-repo
"${CUDA_DOWNLOAD_URL}/${DISTRIBUTION}/${CUDA_ARCH_FOLDER}/cuda-${DISTRIBUTION}.repo"
dnf install -y --nobest --setopt=install_weak_deps=False \
    cuda-nvtx-${version_suffix} cuda-cudart-${version_suffix} \
    libcusolver-${version_suffix} libcublas-${version_suffix}
```

More detailed instructions for your platform can be found in the online documentation of your selected CUDA version. Please make sure to install CUDA version 11.8 or newer, and confirm that your GPU driver supports that version. While the above packages are sufficient to use GPU-acceleration within CUDA Quantum, we recommend installing the complete CUDA toolkit (`cuda-toolkit-11-8`) that also includes the `nvcc` compiler.

Distributed Computing with MPI

CUDA Quantum supports the Message Passing Interface (MPI) parallelism via a plugin interface. It is possible to activate or replace such an MPI plugin without re-installing or re-compiling CUDA Quantum. MPI calls via CUDA Quantum API for C++ and Python will be delegated to the currently activated plugin at runtime.

Built-in MPI Support | Custom MPI Support

The CUDA Quantum Docker image is shipped with a pre-built MPI plugin based on an optimized OpenMPI installation included in the image. No action is required to use this plugin. We recommend using this plugin unless the container host has an existing MPI implementation other than OpenMPI.

If you are not using the Docker image, or are using the image on a system that has a vendor-optimized MPI library pre-installed, please follow the instructions in the "Custom MPI Support" tab to enable MPI support.

Updating CUDA Quantum

If you installed the CUDA Quantum Python wheels, you can update to the latest release by running the command

```
python3 -m pip install --upgrade cuda-quantum
```

If you previously installed the CUDA Quantum pre-built binaries, you should first uninstall your current CUDA Quantum installation before installing the new version using the installer. To uninstall your current CUDA Quantum version, run the command

```
sudo bash "${CUDA_QUANTUM_PATH}/uninstall.sh" -y
```

The `uninstall.sh` script is generated during installation, and will remove all files and folders that were created as part of the installation, whether they were modified in the meantime or not. It does not remove any additional files that existed prior to the installation or that you have added to the installation location since then. You can then download and install the new version of CUDA Quantum following the instructions above.

Dependencies and Compatibility

CUDA Quantum can be used to compile and run quantum programs on a CPU-only system, but a GPU is highly recommended and necessary to use the GPU-based simulators, see also CUDA Quantum Simulation Backends.

The supported CPUs include x86_64 (x86-64-v3 architecture and newer) and ARM64 architectures.

Note

Some of the components included in the CUDA Quantum Python wheels depend on an existing CUDA installation on your system. For more information about installing the CUDA Quantum Python wheels, take a look at this section.

The following table summarizes the required components.

Supported Systems

CPU architectures	x86_64, ARM64
Operating System	Linux
Tested Distributions	CentOS 8; Debian 11, 12; Fedora 38; OpenSUSE/SLED/SLES 15.5; RHEL 8, 9; Rocky 8, 9; Ubuntu 22.04
Python versions	3.8+

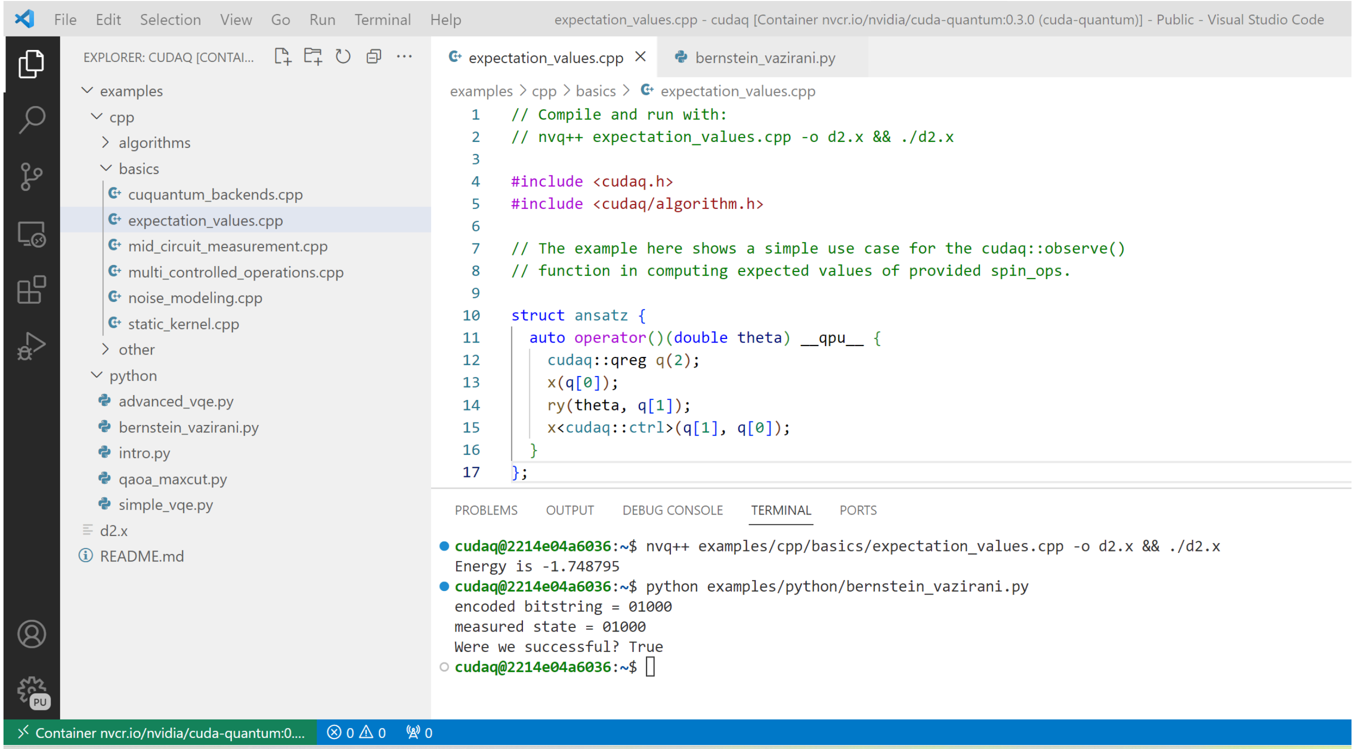
Requirements for GPU Simulation

GPU Architectures	Volta, Turing, Ampere, Ada, Hopper
NVIDIA GPU with Compute Capability	7.0+
CUDA	11.x (Driver 470.57.02+), 12.x (Driver 525.60.13+)

Detailed information about supported drivers for different CUDA versions and be found here.

Next Steps

You can now compile and/or run the C++ and Python examples using the terminal. To open a terminal in VS Code, open the Command Palette with `Ctrl+Shift+P` and enter “View: Show Terminal”.



The CUDA Quantum image contains a folder with examples and tutorials in the `/home/cudaq` directory. These examples are provided to get you started with CUDA Quantum and understanding the programming and execution model. If you are not using a container image, you can find these examples on our GitHub repository.

Let's start by running a simple program to validate your installation. The samples contain an implementation of a Bernstein-Vazirani algorithm. To run the example, execute the command:

Python C++

```
python examples/python/bernstein_vazirani.py --size 5
```

This will execute the program on the default simulator, which will use GPU-acceleration if a suitable GPU has been detected. To confirm that the GPU acceleration works, you can increase the size of the secret string, and pass the target as a command line argument:

Python C++

```
python examples/python/bernstein_vazirani.py --size 25 --target nvidia
```

This program should complete fairly quickly. Depending on the available memory on your GPU, you can set the size of the secret string to up to 28-32 when running on the `nvidia` target.

Note

If you get an error that the CUDA driver version is insufficient or no GPU has been detected, check that you have enabled GPU support when launching the container by passing the `--gpus all` flag (for Docker) or the `--nv` flag (for Singularity). If you are not running a container, you can execute the command `nvidia-smi` to confirm your setup; if the command is unknown or fails, you do not have a GPU or do not have a driver installed. If the command succeeds, please confirm that your CUDA and driver version matches the supported versions.

Let's compare that to using only your CPU:

Python C++

```
python examples/python/bernstein_vazirani.py --size 25 --target qpp-cpu
```

When you execute this command, the program simply seems to hang; that is because it takes a long time for the CPU-only backend to simulate 28+ qubits! Cancel the execution with `Ctrl+C`.

You are now all set to start developing quantum applications using CUDA Quantum! Please proceed to Basics for an introduction to the fundamental features of CUDA Quantum.