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Chapter 1. DGL Overview

The NVIDIA® Deep Learning SDK accelerates widely-used deep learning frameworks such as DGL. DGL is an easy-to-use, high performance and scalable Python package for deep learning on graphs. DGL is framework agnostic, meaning if a deep graph model is a component of an end-to-end application, the rest of the logics can be implemented in any major frameworks, such as PyTorch, Apache MXNet, or TensorFlow.

There are two containers available:

- **DGL container** - consists of the latest versions of DGL and PyTorch, their dependencies, and the latest performance optimizations to run your code with GPU-accelerated performance immediately.

- **SE(3)-Transformer for DGL container** - accelerated neural network training environment based on DGL, SE(3)-Transformer, and PyTorch and suited for recognizing 3-dimensional shapes.
  
  This is useful for segmenting LIDAR point clouds or in pharmaceutical and drug discovery research, for example.

The GPU-accelerated NVIDIA DGL containers help developers and data scientists who work with Graph Neural Networks (GNN) on large, heterogeneous graphs with billions of edges. These containers allow developers to work more efficiently in an integrated, GPU-accelerated environment that combines DGL and PyTorch. Instead of using home-grown software that is expensive to maintain, developers can use end-to-end GNN solutions through tested, validated, and supported containers.

This document describes the key features, software enhancements and improvements, known issues, and how to run this container.
Chapter 2. Pulling A Container

About this task

Release 23.07 is based on CUDA 12.1.1, which requires NVIDIA Driver release 530 or later. However, if you are running on a data center GPU (for example, T4 or any other data center GPU), you can use NVIDIA driver release 450.51 (or later R450), 470.57 (or later R470), 510.47 (or later R510), 515.65 (or later R515), 525.85 (or later R525), or 530.30 (or later R530).

The CUDA driver’s compatibility package only supports particular drivers. Thus, users should upgrade from all R418, R440, R460, and R520 drivers, which are not forward-compatible with CUDA 12.1. For a complete list of supported drivers, see the CUDA Application Compatibility topic. For more information, see CUDA Compatibility and Upgrades.

Before you can pull a container from the NGC container registry:

- Install Docker.
  - For NVIDIA DGX™ users, see Preparing to use NVIDIA Containers Getting Started Guide.
  - For non-DGX users, see NVIDIA® GPU Cloud™ (NGC) container registry installation documentation based on your platform.
- Ensure that you have an NGC API Key to log in to the NGC container registry.
  Refer to NGC Getting Started Guide for more information.
Chapter 3. Running DGL

Before you can run an NGC deep learning framework container, your Docker environment must support NVIDIA GPUs. To run a container, issue the appropriate command as explained in Running A Container and specify the registry, repository, and tags.

On a system with GPU support for NGC containers, when you run a container, the following occurs when running a container:

- The Docker engine loads the image into a container that runs the software.
- You define the container’s runtime resources by including the additional flags and settings that are used with the command.
  
  These flags and settings are described in Running A Container.
- The GPUs are explicitly defined for the Docker® container, which defaults to all GPUs, but can be specified by using the NVIDIA_VISIBLE_DEVICES environment variable.

  For more information, refer to the nvidia-docker documentation.

  Note: Starting in Docker 19.03, complete the steps below.

The method implemented in your system depends on the DGX OS version installed (for DGX systems), the specific NGC Cloud Image provided by a Cloud Service Provider, or the software that you have installed in preparation for running NGC containers on TITAN PCs, Quadro PCs, or vGPUs.

1. Issue the command for the applicable release of the container that you want.
   
   The following command assumes you want to pull the latest container:
   
   `docker pull nvcr.io/nvidia/dgl:<xx.xx>-py3`

2. Open a command prompt and paste the pull command.
   
   Ensure that the pull process completes successfully before proceeding to step 3.

3. Run the container image.
To run the container, select one of the following modes:

- **Interactive mode:**
  
  If you have **Docker 19.03 or later**, a typical command to launch the container is:
  
  ```bash
docker run --gpus all --it --rm -v local_dir:container_dir nvcr.io/nvidia/dgl:<xx.xx>-py3
  ```
  
  If you have **Docker 19.02 or earlier**, a typical command to launch the container is:
  
  ```bash
  nvidia-docker run --it --rm -v local_dir:container_dir nvcr.io/nvidia/dgl:<xx.xx>-py3
  ```

- **Non-interactive mode:**

  If you have **Docker 19.03 or later**, a typical command to launch the container is:
  
  ```bash
docker run --gpus all --rm -v local_dir:container_dir nvcr.io/nvidia/dgl:<xx.xx>-py3
  ```
  
  If you have **Docker 19.02 or earlier**, a typical command to launch the container is:
  
  ```bash
  nvidia-docker run --rm -v local_dir:container_dir nvcr.io/nvidia/dgl:<xx.xx>-py3
  ```

  **Note:** If you use multiprocessing for multi-threaded data loaders, the default shared memory segment size that the container runs with might not be enough. To increase the shared memory size, run one of the following commands:
  
  ```bash
  --ipc=host
  ```
  or
  
  ```bash
  --shm-size=<requested memory size>
  ```
  in the command line to
  
  ```bash
docker run --gpus all
  ```

You might want to pull data and model descriptions from locations outside the container for use by DGL or save results to locations outside the container. The easiest method is to mount one or more host directories as Docker **data volumes**.
Chapter 4. DGL Release 23.07

The NVIDIA container image for DGL, release 23.07, is available on NGC.

Contents of the DGL container

This container image contains the complete source of the version of DGL in /opt/dgl/dgl-source. It is pre-built and installed as a system Python module.

The container includes the following:

- DGL 1.1+f635e2a
- PyTorch 23.07
- RAPIDS 23.06
- Ubuntu 20.04 including Python 3.8
- NVIDIA CUDA® 12.1.1
- NVIDIA cuBLAS 12.1.3.1
- NVIDIA cuDNN 8.9.3
- NVIDIA NCCL 2.18.3
- Apex
- rdma-core 39.0
- OpenMPI 4.1.4+
- GDRCopy 2.3
- Nsight Compute 2023.1.1.4
- Nsight Systems 2023.2.3.1001
- NVIDIA HPC-X 2.15
- TensorRT 8.6.1.6
- SHARP 2.5
- TensorBoard 2.7.0
- DALI 1.27.0
GPU Requirements

Release 23.07 supports CUDA compute capability 6.0 and later. This corresponds to GPUs in the NVIDIA Pascal, NVIDIA Volta™, NVIDIA Turing™, NVIDIA Ampere architecture, and NVIDIA Hopper™ architecture families. For a list of GPUs to which this compute capability corresponds, see CUDA GPUs. For additional support details, see Deep Learning Frameworks Support Matrix.

Key Features and Enhancements

This DGL release includes the following key features and enhancements.

‣ DGL container image version 23.07 is based on DGL 1.1.1.

The major features of the release can be found in the DGL release notes.

Announcements

None.

NVIDIA DGL Container Versions

The following table shows what versions of Ubuntu, CUDA, DGL, and TensorRT are supported in each NVIDIA containers for DGL. For older container versions, refer to the Frameworks Support Matrix.

<table>
<thead>
<tr>
<th>Container Version</th>
<th>Ubuntu</th>
<th>CUDA Toolkit</th>
<th>DGL</th>
<th>PyTorch</th>
</tr>
</thead>
<tbody>
<tr>
<td>23.07</td>
<td>22.04</td>
<td>NVIDIA CUDA 12.1.1</td>
<td>0.9.x</td>
<td>23.07</td>
</tr>
</tbody>
</table>

Known Issues

‣ The tensors that are used as node features must be contiguous and cannot be views of other tensors when the use_uva flag is set to True in the dgl.dataloading.Dataloader class.

When you attempt to use a graph with a non-contiguous or view tensors for edata or ndata, a DGLError will occur.
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