NVIDIA Topology-Aware GPU Selection 0.1.0 (Early Access)

User Guide

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Table of Contents

List of Tables

Chapter 1. Introduction

Many NVIDIA® graphical processing units (GPU)-accelerated HPC applications that use Message Passing Interface (MPI) spend a substantial portion of their runtime in non-uniform GPU-to-GPU communications. These expensive communications prevent users from maximizing performance from their existing hardware.

To ensure that GPU-to-GPU communication in these applications is efficient, you need to make informed decisions when assigning GPUs to MPI processes. The assigning of GPUs to processes depends on the following factors:

- System GPU topology

  Shows how different GPUs are linked and the communication channel they use to connect. Different communication channels exist in multi-GPU servers, which results in some GPU pairs using faster communication links than other GPU pairs.
- Application GPU profiling

  Shows the total volume of communication between different GPUs in the system. This topology shows the application's communication pattern and also shows that some GPU pairs can have a higher communication volume than other pairs.

NVIDIA® Topology-Aware GPU Selection (NVTAGS) is a toolset for high performance computing (HPC) applications that uses MPI to enable faster solve times for applications with a high GPU communication time and a communication pattern that does not fit the underlying system GPU topology.

NVTAGS does the following:

- Profiles application GPU communication by using a PMPI-based profiler.
- Extracts system GPU communication topology that leverages NVIDIA's System Management Interface (nvidia-smi).
- Finds an efficient way of assigning GPUs to processes to minimize GPU communication congestion.
- Intelligently and automatically assigns GPUs to MPI processes.

  This reduces the overall GPU-to-GPU communication time of HPC applications that run on a multi-GPU system.

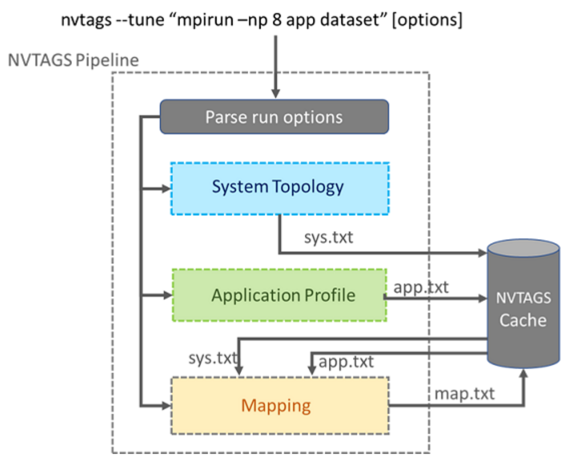
Here is the two-step process that NVTAGS follows to identify and apply efficient GPU assignments:

1. NVTAGS Tune

In this step, NVTAGS does the following:

- Gathers, or uses already available, application and system profiling data to understand how GPU-to-GPU communication is performed for a target application.
- Leverages this profiling information to identify and recommend a GPU assignment solution that better suits your application on the target system, so this assignment solution can be used in subsequent runs.

The following figure shows the NVTAGS tuning pipeline and the workflow to find an efficient GPU assignment. As you can see, the system GPU topology and application GPU profiling are extracted and cached in the `sys.txt` and the `app.txt` files. These files are fed to the NVTAGS mapping component and are used by a graph mapping algorithm to look for a better GPU assignment and store the result in the `map.txt` file in the NVTAGS cache.



2. NVTAGS Run

   In this step, NVTAGS applies the suggested GPU assignment from the tuning step and initiates your application run command. Optionally, based on how GPUs are selected in your application, NVTAGS also automatically sets the proper CPU and NIC affinity.

> Note: Both NVTAGS Tune and Run steps are light weight and impose negligible overhead for most of the MPI applications.

Systems that NVTAGS Benefits

NVTAGS leverages the GPU communication pattern of an application and the GPU topology of a system to generate efficient GPU assignments for an application that runs on the system.

NVTAGS benefits systems with asymmetric system topologies where some GPU pairs share stronger communication links than other pairs. Examples of these systems include NVIDIA DGX-1™ and PCIe servers that use different GPU communication channels to connect GPUs. Systems with symmetric system topologies, where all GPU pairs use the same communication links with equal capacity, will not benefit from custom GPU assignment because shuffling GPUs do not guide processes to use GPU pairs with stronger communication links. Examples of thse systems include NVIDIA DGX-2™ and NVIDIA DGX™ A100. Systems with symmetric topologies do not benefit from NVTAGS because all GPU assignments on such systems are equally optimal.

Chapter 2. Getting Started

This section provides information about the requirements to install NVTAGS, the installation instructions, and how to use NVTAGS.

2.1. Prerequisites

This section provides information about installing and using NVTAGS.

Ensure that you have completed the following prerequisites:

- Have a Linux operating system.
- Have an x86 system architecture.
- Installed a working NVIDIA Graphics Driver.

  To download the driver, go to Download Drivers.
- Have at least 3 GPUs installed on your machine.
- Verified that your application uses one GPU per MPI process and runs with at least 3 processes (3 GPUs).
- Have a CUDA-aware Open MPI to run your application.
- Verified that your Open MPI version matches the NVTAGS profiler library version.

  A different version might work but is not recommended. NVTAGS currently includes a profiler library that supports Open MPI 4.0.
- Optional: If you decide to use NVTAGS with CPU binding, `numactl` needs to be available on your machine.

  Depending on your OS, `numactl` can be installed by using `apt-get install numactl` , `yum install numactl` or other method.

2.2. Installing NVTAGS

Complete these steps to install NVTAGS.

About this task

Before you install NVTAGS, read Prerequisites.

Procedure

1. Download the latest NVTAGS release from the NVTAGS releases page.
2. To extract the NVTAGS archive, run:
```
tar -xzvf nvtags-ea-0.1.0.tar.gz
```
3. Copy the NVTAGS directory into the default NVTAGS path on your machine:
```
cp -r nvtags-ea-0.1.0 /opt/nvtags
```
4. Update `PATH` to make the NVTAGS binaries discoverable:
```
export PATH=/opt/nvtags/bin:${PATH}
```
5. (Optional) Although the NVTAGS binaries and scripts that are bundled in the NVTAGS release archive are executable, depending on your system, you might need to update your permissions.
```
chmod +x /opt/nvtags/bin/*
```
6. (Optional) If you do not have permission to copy the NVTAGS package into `/opt/nvtags/`, complete the following tasks:
   a). Adjust `PATH` to point to the NVTAGS binaries on the appropriate path.
   b). Set `NVTAGS_DEF_LIB_DIR` to a directory path where the NVTAGS library (for example, `libmpi_prof_x.y.so` or `libmpi_prof.so`) exists.
```
export PATH=/MY/PATH/TO/nvtags/bin:${PATH}
export NVTAGS_DEF_LIB_DIR=/MY/PATH/TO/nvtags/libs
```

Chapter 3. Using NVTAGS

This section provides additional information about the two NVTAG modes, NVTAGS Tune and NVTAGS Run.

3.1. NVTAGS Tune Mode

In the NVTAGS Tune mode, the application and system profiling data is used to recommend an efficient GPU assignment.

The Tune mode requires application profiling data to evaluate the efficiency of default GPU assignments and search for a better GPU assignment by using mapping algorithms. Depending on whether application profiling data exists, tuning can be completed with or without profiling.

After the tuning is complete, subsequent application runs can be used with NVTAGS in the Run mode.

3.1.1. Tune with profiling

To tune with profiling, application profiling data is used to extract the GPU communication pattern of the application.

If you do not know the GPU communication pattern, NVTAGS must be used in the Tune with profiling mode. You can also manually provide the pattern and use the Tune without profiling option. See Tune without Profiling for more information.

NVTAGs uses an MPI profiler library that dynamically links to your MPI application and intercepts MPI calls to build a GPU communication pattern. After the profiling is complete, NVTAGS looks for a better GPU assignment solution by using the application and system GPU topology information. The profiling results and recommended GPU assignments are cached in the local NVTAGS cache that defaults to `./.nvtags/.cache`.

Although NVTAGS can provide an efficient GPU assignment by using the default settings, NVTYAGS might provide a better GPU assignment by using non-default settings. This process can be achieved by changing the default profiling and mapping settings with input arguments. The profiling information is cached after each tuning step, so when you tune the settings again, you do not need to profile your application again. See About the NVTAGS CLI for more information.

3.1.2. Run NVTAGS in Tune with Profiling Mode

You can run NVTAGS in Tune with Profiling mode.

Procedure

To run NVTAGS in the Tune with Profiling mode, prepend your application run command with `nvtags --tune`:

```
nvtags [options] --tune "application run cmd"
```

3.2. Tune NVTAGS without Profiling Mode

You can run NVTAGS in Tune without Profiling mode.

After the application profiling data is available once, if a better GPU assignment exists, you can search for this assignment by using the cached data and without profiling your application again. NVTAGS runs quickly in this mode because it already has access to the profiling data for your application.

NVTAGS supports different mapping and profiling options, and if an efficient mapping exists, the default options usually successfully finds it. However, this might not be the case for all applications. For complete list of mapping and profiling options check Mapping Options and Application Profiling Options.

When the tuning step is complete, and a better GPU assignment is found, a message similar to the following is printed. A list of GPU IDs is stored in the `.nvtags/.cache/map.txt` file.

```
Better mapping found!
Max Congestion_improvement: 10.00%
Avg Congestion_improvement: 17.27%
0,1,3,2,7,6,4,5
```

> Note: GPU IDs are only stored when the congestion improvement is greater than the NVTAGS threshold value. The default value is 5%.

If no better GPU assignment is found, nothing is stored in the `.nvtags/.cache/map.txt` file, and NVTAGS outputs the following message:

```
No Better mapping found!
```

3.2.1. Run NVTAGS in Tune without Profiling Mode

You can tune NVTAGS in Tune without Profiling Mode.

Procedure

To tune NVTAGS without profiling, use the `--rebuild-prof` option:

```
nvtags [options] --rebuild-prof
```

3.3. NVTAGS Run Mode

Here is some information about the NVTAGS Run mode.

In the Run mode, NVTAGS applies the recommended efficient GPU assignment from the tuning process by setting `CUDA_VISIBLE_DEVICES` and executing your application run command. NVTAGS can also pin the CPU and the NIC based on their affinity information and the GPU assignment.

3.3.1. Run Mode with Binding

You can configure automatic CPU and NIC binding by using the `nvtags_run.sh` script, which can be found in the `/opt/nvtags/bin/nvtags_run.sh` directory.

This script automatically detects the CPU and NIC affinity, and based on the GPU assignment, binds them to each process.

Here is an example of how to apply NVTAGS to the `mpirun -np 8 app args` run command:

```
mpirun -np 8 --bind-to none -x EXE=app -x ARGS=args nvtags_run.sh
```

> Note: To run NVTAGS in this mode:
>
> - Pass the `--bind-to none` flag to the `mpirun` command, so that MPI does not attempt to handle the setting affinity.
> - Ensure that `numactl` is available on your system.

3.3.2. Run NVTAGS in Run Mode without Binding

You can run NVTAGs in Run mode without binding.

Procedure

To run your application with NVTAGS, add `nvtags --run` before your application run command:

For example:

```
nvtags [options] --run "application run cmd"
```

In this mode, there is no CPU or NIC pinning.

3.4. About the NVTAGS CLI

This section provides additional information about the two NVTAGS modes, NVTAGS Tune and NVTAGS Run.

3.4.1. CLI Options for the Tune Mode

You can tune the CLI with or without profiling.

Procedure

Complete one of the following options:

- To tune with application profiling, use the `--tune` option and pass the application run command to it.

  ```
  nvtags [options] --tune application run cmd  # tune with profiling
  ```

- To tune without application profiling, and use the existing cached data, run the `--rebuild-prof` option.

  ```
  nvtags [options] --rebuild-prof    # tune without profiling
  ```

3.4.1.1. System profiling options

Here is some information about the options that are used to modify NVTAGS system profiling parameters.

The system profiling options are `-m, --manual` .

By default, NVTAGS assigns predefined values to system GPU communication channels, which are calculated by using the channels' bandwidth and latency. Table 1 shows the list of GPU links that are recognized by `nvidia-smi` and their corresponding default values.

To better represent the strength of the communication links on your system, you can modify these values by setting the environment variable that NVTAGS associates with the link. The environment variable name that is used by NVTAGS is constructed by adding `NVTAGS_PROF_` to the name of the link. For example, `NVTAGS_PROF_SYS` is used to change the SYS default link value, and `NVTAGS_PROF_NV1` is used to change the NV1 default link value.

3.4.1.2. Supported Link Names

This table provides a list of the supported link names and their default values.

Table 1. List of Supported Link Names in NVTAGS and their Default Value and Description

Link Name	Link Description	Link Value
SYS	Connection traversing the PCIe and SMP interconnect	10

Link Name	Link Description	Link Value
	between NUMA nodes (Inter-socket)	
NODE	Connection traversing the PCIe and interconnect between Host Bridges in a NUMA node	19
PHB	Connection traversing PCIe and a PCIe Host Bridge	18
PXB	Connection traversing multiple PCIe bridges without traversing the Host Bridge	20
PIX	Connection traversing a maximum of one PCIe bridge	20
NV1	Connection traversing a bonded set of 1 NVLinks	25
NV2	Connection traversing a bonded set of 2 NVLinks	25
NV3	Connection traversing a bonded set of 3 NVLinks	25
NV4	Connection traversing a bonded set of 4 NVLinks	25
NV5	Connection traversing a bonded set of 5 NVLinks	25
NV6	Connection traversing a bonded set of 6 NVLinks	25
NV12	Connection traversing a bonded set of 6 NVLinks	25

After you set your new values to the link names by using their environment variables, use the `--manual` argument so their values can be applied by NVTAGS.

Although NV1 to NV12 have different bandwidth capacities, experiments on various systems and MPI applications shows that using the same value for all NVLinks leads to better mapping results. The mapping algorithm uses this value to select NVLinks, over non-NVLinks instead of selecting NVLinks with different bonded sets over each other. If it does not apply to your application and/or system, you can use a manual assignment to change the default link values.

3.4.1.3. Application Profiling Options

This section provides information about the options that are used to modify the application profiling parameters.

`-d, --disable-normalized:`

By default, NVTAGS normalizes raw application GPU communication pattern values, represented in bytes, because some mapping algorithms work better when normalized values are used. To disable this feature, and use raw communication pattern values, pass `--disable-normalize` (or `-d`) to the NVTAGS Tune command.

`-e, --enable-symmetric:`

This option allows you to make application profiling values symmetric. By default, application communication patterns are not symmetric, but sometimes mapping algorithms can find a better solution if a symmetric profiling value is used.

`-f, --prof-lib-path <path to dir>`

By default, NVTAGS uses a default porfiler that exists in the `/opt/nvtags/libs` directory or in the directory that is set by `NVTAGS_DEF_LIB_DIR`. However, you can provide the exact path to your custom profiler by using the `-prof-lib-path` argument with the profiler path.

`-v, ---normalized-value <value>`

The default normalization value is 100, which results in scaling raw GPU communication data that ranges between 0 and 100. You can change this default normalization value by using the `--normalized-value (or -v)` argument with the new value.

3.4.1.4. Mapping Options

These mapping group options can be used to modify mapping parameters.

`-i, --improvement-threshold`

NVTAGS uses a congestion metric to compare new GPU assignment candidates against your application's default assignment. Only GPU assignments that can improve the default assignment congestion by more than the threshold value are stored. By default, this threshold value is set to 5%, but it can be changed by using the `--improvement` (or `-i`) argument with the new threshold value. The new value must be between 0 and 100.

`-m, --map-alg map alg name`

Here are the options for the *map alg name* variable:

- **`greedy`**
- **`rb`**
- **`all`**

Currently, NVTAGS supports the Greedy (**`greedy`**), Recursive-bipartitioning (**`rb`**), and All (**`all`**) mapping algorithms. The `All` mapping algorithm is the default mapping, which is a combination of the `Greedy` and `RB` algorithms. You can change the `All` mapping algorithm to the `RB` or the `Greedy` algorithm by using `--map-alg` (or `-m`) and the mapping name.

`-o, --opt-time time in ms`

By default, NVTAGS spends 1000 ms (1 second) to evaluate and optimize different mapping solutions. If an efficient GPU assignment solution exists, the solution is found during this period. To change this value, use the `--opt-time` (or `-o`) argument with the new optimization period.

3.4.2. CLI options for the Run Mode

This section provides information about the CLI options that you can use to run NVTAGS in Run mode with or without binding.

- To run NVTAGS with the binding, use the `nvtags_run.sh` script.
- To run NVTAGS without binding, use the NVTAGS binary.

3.4.2.1. Run Mode with the Binding CLI

To use the NVTAGS Run mode with binding, pass the application run command to the `nvtags_run.sh` script.

To run the script, you must set the `EXE` and `ARGS` values to the application executable and other application arguments. For example, to run the `mpirun -np 8 app all other args` command with `nvtags_run.sh` script, run the following command:

```
mpirun -np 8 --bind-to none -x EXE="app" -x ARGS="all other args" nvtags_run.sh
```

This script reads the new potential GPU assignment from the `./.nvtags/.cache/map.txt` file and, before starting the application run command, sets `CUDA_VISIBLE_DEVICES`. It also extracts the system affinity information and the CPU and NIC affinity setting. By default, this script uses 1 thread per process and binds the process to core. When you run the script by using `N` processes, the script assumes that you are using `GPU 0` to `GPU N-1` on your system. You can change these default values by setting the associated environment variables before running your application.

- To change the number of threads, before running the NVTAGS run commend, set `OMP_NUM_THREADS`.
- To change the bind target, set `NVTAGS_BIND_TARGET` to `socket` (for socket binding) or `core` (for core binding).
- To change the GPU list that your application uses, set `NVTAGS_GPU_LIST` to comma-separated list of GPUs.

Note: By default, applications use `GPU0` to `GPU N-1` when running with the `N` process. You do not need to change this environment variable frequently.

3.4.2.2. Examples

Here are some examples of running NVTAGS in Run mode with binding.

Example: Use NVTAGS Run with Binding to the Socket

Here is an example where the Run mode is used with binding to `socket`:

```
export NVTAGS_BIND_TARGET=socket
```

```
mpirun -np 8 --bind-to none -x EXE="app" -x ARGS="all other args" nvtags_run.sh
```

Example: Use NVTAGS Run with Binding to Core using Four Threads per Process

Here is an example where the Run mode is used with binding to `core`:

```
export NVTAGS_BIND_TARGET=core
export OMP_NUM_THREADS=4
mpirun -np 8 --bind-to none -x EXE="app" -x ARGS="all other args" nvtags_run.sh
```

If NVTAGS cannot find a better mapping in the tuning step, running the `nvtags_run.sh` script exits the process. Since no mapping file exists, by default, the application will not run.

To change this behavior and allow NVTAGS to run your application with the default GPU assignment and apply CPU and NIC bindings, before you run the `nvtags_run.sh` script, set `NVTAGS_ALLOW_DEFAULT_RUN` to **1**.

3.4.2.3. Run Mode without the Binding CLI

You can use the Run mode with the binding CLI.

To use NVTAGS without binding, pass the application run command to the `--run` argument. If no mapping file is found from the tuning step, and there is no binding CLI, NVTAGS will not run the application.

To change this behavior and allow the application to run NVTAGS with the default GPU assignment, set `NVTAGS_ALLOW_DEFAULT_RUN` to **1**.

3.5. Generic CLI Options

Here is a list of generic options that can be used with the NVTAGS binary in the Tune and Run modes.

`-h, --help`

Prints a help message that includes a description of how to use NVTAGS and its options.

`-l, --log-level`

Enables debug logs that are, by default, disabled. To enable the logs, use the `--log-level` DEBUG option.

`-p, --path`

The path to a directory where NVTAGS caches the profiling and mapping files. The default path is `./nvtags/.cache/`.

Chapter 4. NVTAGS Examples

This section contains information and sample code to help you understand NVTAGS.

4.1. Examples: NVTAGS Tune Mode

The following examples show a variety of tuning options.

Tune with Profiling

Example 1: Tune `app2` with `dataset2` by using the default tuning options with a normalization value of `50`:

```
nvtags --tune "mpirun -np 8 app dataset" --normalized-value 50
```

Tune Without Profiling

Example 2: Using the cached profiling data in Example 2, complete retuning for `app2` with a normalization value of `200`:

```
nvtags --rebuild-prof --normalized-value 200
```

Tune with Custom Profiling Options

Example 3: Tune `app3` with `args3` by using custom manual system profiling link values. In this example, a DGX-1 server is used with the `SYS`, `NV1`, `NV2` link names, and you want to manually assign `1`, `2`, and `3` to these names:

```
export NVTAGS_PROF_SYS=1
export NVTAGS_PROF_NV1=2
export NVTAGS_PROF_NV2=3
nvtags --tune "mpirun -np 8 app3 args3" --manual
```

Tune with Custom Mapping Options

Example 4: Tune `app4` with `dataset4` by using symmetric, not normalized, application profiling with an improvement threshold value of `2.5`%:

```
nvtags --tune "mpirun -np 8 app4 dataset4" --disable-normalized --enable-symmetric
 --improvement-threshold 2.5
```

Example 5: Retune `app4` from *Example 4* by changing the default mapping to `"greedy"` and the optimization time to `3000` milliseconds (3 seconds):

> Note: When retuning an app, navigate to the same folder where you previously tuned the app. This step ensures that the `./.nvtags/.cache` directory content from the previous tuning is accessible.

```
nvtags --rebuild-prof --map-alg "greedy" --opt-time 3000
```

Tune with the Custom Cache Path

Example 6: Tune `app5` with `dataset5` by using the custom NVTAGS cache path:

```
nvtags "mpirun -np 8 app5 dataset5" --path /home/nvtags/mycache
```

When you use custom cache for tuning, if you do not provide the custom cache path, the default cache path is selected during an NVTAGS run:

```
nvtags "mpirun -np 8 app5 dataset5" --path /home/nvtags/mycache
```

4.2. Examples: NVTAGS Run Mode with Binding

Here are some examples that show the Run mode with binding.

In this mode, by using the `nvtags_run.sh` script, `CUDA_VISIBLE_DEVICES` is set by using the `./nvtags/.cache/map.txt` content, and `CUDA_VISIBLE_DEVICES` is based on new GPU assignment. This assignment is also used to perform CPU and NIC pinning based on their affinity information.

Example 7: Run `app4` with `dataset4` (tuned in *Example 6* in Examples: NVTAGS Tune Mode) by using the default setting. This setting binds the CPUs to core and uses 1 thread per CPU core:

```
mpirun -np 8 --bind-to none -x EXE="app4" -x ARGS="dataset4" nvtags_run.sh
```

Example 8: Run `app4` with `dataset4` (tuned in *Example 6* in Examples: NVTAGS Tune Mode) using socket for binding:

```
export NVTAGS_BIND_TARGET=socket
mpirun -np 8 --bind-to none -x EXE="app4" -x ARGS="dataset4" nvtags_run.sh
```

Example 9: Run `app4` with `dataset4` (tuned in *Example 6* in Examples: NVTAGS Tune Mode) using core binding and 4 threads per process:

```
export NVTAGS_BIND_TARGET=core
export OMP_NUM_THREADS=4
mpirun -np 8 --bind-to none -x EXE="app4" -x ARGS="dataset4" nvtags_run.sh
```

In this mode, when a better GPU assignment is found from previous step(s) in the `./nvtags/.cache/map.txt` file, `CUDA_VISIBLE_DEVICES` is set before starting the application command. Otherwise, NVTAGS skips running the application unless `NVTAGS_ALLOW_DEFAULT_RUN` is set to 1.

Example 10: Run `app4` with `dataset4` (tuned in *Example 6* in Examples: NVTAGS Tune Mode) with the log-level debug:

```
nvtags --run "mpirun -np 8 app dataset" --log-level debug
```

4.3. End-to-End Usage Example

This section includes an example to complete NVTAGS tuning and running with the Jacobi kernel.

Here is the standard Jacobi run command for this example:

```
mpirun -np 8 ./jacobi -t 4 2
```

NVTAGS Tune

1. Run the tuning step to profile your application and system topology:

   ```
   nvtags --tune "mpirun -np 8 ./jacobi -t 4 2"
   ```

2. Review the logs that indicate by how much communication congestion will improve with the NVTAGS-recommended GPU assignment:

   ```
   NVTAGS: 2020-06-16 08:36:07 info : Detected number of processes from profiling
    file is "8"!
   NVTAGS: 2020-06-16 08:36:08 info : Better mapping found!
   NVTAGS: 2020-06-16 08:36:08 info : Max Congestion improvement: 0.00%
   NVTAGS: 2020-06-16 08:36:08 info : Avg Congestion improvement: 11.54%
   NVTAGS: 2020-06-16 08:36:08 info : mapping result is stored in "./.nvtags/.cache/
   map.txt"!
   ```

NVTAGS Run

To launch your application with the improved GPU assignment that was recommended by NVTAGS:

Run Mode with CPU/NIC binding

```
mpirun -np 8 --bind-to none -x EXE="./jacobi" -x ARGS="-t 4 2" nvtags_run.sh
```

Run Mode without Binding

```
nvtags --run "mpirun -np 8 ./jacobi -t 4 2"
```

Chapter 5. Licensing

This section includes the license for NVTAGS and some third-party licenses.

5.1. NVTAGS License

Here is the license for NVTAGS.

```
Apache License
 Version 2.0, January 2004
 http://www.apache.org/licenses/

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