Installing NetCDF with NVIDIA HPC SDK (NVHPC)

This repository (or directory) contains the tools and scripts needed to install the **NetCDF** scientific stack **(C and Fortran)** using **NVIDIA** compilers **(nvfortran and nvc)** on Linux systems (Ubuntu/Debian or RHEL/CentOS).

🏷️ Prerequisites

The installer automates most dependencies, but the following is assumed:

- **Operating System:** Ubuntu 24.04 LTS (tested) or RHEL-based distributions.
- **Privileges:** Access to sudo to install system packages and write to /usr/local or /opt.
- **Disk Space:** At least **20GB** free is recommended (the NVIDIA installer takes up ~15GB compressed and ~7GB installed).

🚀 Quick Installation Guide

1. **Run the installation script:**

   Bash

   ```
   sudo ./install_netcdf_nvhpc.sh
   ```

2. **Configure the path:** When prompted by the script, press Enter to use the default path: /usr/local/netcdf-nvfortran.

The script will perform the following actions:

- Detect and install dependencies (m4, make, libxml2, hdf5-serial).
- Download and install **NVHPC 26.1** if it is not detected on the system.
- Compile **NetCDF-C 4.9.2** with support for HDF5.
- It will compile **NetCDF-Fortran 4.6.1** linking to the previous C library.

🛠️ Environment Configuration

To use the compilers and libraries, add the following lines to your ~/.bashrc (or ~/.zshrc) file:

Bash

```
# NVIDIA HPC SDK
export NV_ROOT=/opt/nvidia/hpc_sdk/Linux_x86_64/26.1/compilers export
PATH=$NV_ROOT/bin:$PATH
export LD_LIBRARY_PATH=$NV_ROOT/lib:$LD_LIBRARY_PATH

# NetCDF-Fortran
export NC_ROOT=/usr/local/netcdf-nvfortran export
PATH=$NC_ROOT/bin:$PATH
export LD_LIBRARY_PATH=$NC_ROOT/lib:$LD_LIBRARY_PATH
```

Then, reload your terminal: source ~/.bashrc.

□ Verification Tests

To confirm that the installation is correct and that nvfortran can link the library, follow these steps:

1. Verify binaries

Run the following commands to confirm that the tools respond:

Bash

```
nvfortran --version
nf-config --version
```

2. Compilation test (Hello NetCDF)

Create a file named test_nc.f90:

Fortran

```
program test_netcdf
    use netcdf
    implicit none
    integer :: ncid, status

    status = nf90_create('test_output.nc', NF90_CLOBBER, ncid) if
    (status /= nf90_noerr) then
        print *, "Error creating file:", nf90_strerror(status) stop 1
    end if

    status = nf90_close(ncid)
    print *, "Success! NetCDF-Fortran and NVHPC are linked correctly." end program
test_netcdf
```

3. Compile and run

Use the nf-config utility to automatically obtain the compilation flags:

Bash

```
nvfortran test_nc.f90 -o test_nc $(nf-config --fflags --flibs)
./test_nc
```

Generated Path Structure

Component	Installation Path
NVHPC SDK	/opt/nvidia/hpc_sdk/
NetCDF Binaries	/usr/local/netcdf-nvfortran/bin/
NetCDF Includes	/usr/local/netcdf-nvfortran/include/
NetCDF Libraries	/usr/local/netcdf-nvfortran/lib/

⚠ Troubleshooting Common Problems

- **Error: relocation R_X86_64_32S**: This error occurs if -fPIC is not used. The installation script already forces this flag, but if you manually compile other programs, be sure to include it.
- **Error: Can't find or link to hdf5**: On Ubuntu 24.04, the script specifically targets /usr/include/hdf5/serial. If you are using a custom HDF5 installation, you will need to adjust the CPPFLAGS and LDFLAGS in the script.