NVIDIA Nsight Systems

The Delta documentation has moved to https://docs.ncsa.illinois.edu/systems/delta/. Please update any bookmarks you may have. Click in the link above if you are not automatically redirected in 5 seconds.

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- Python with NVTX
 - o Install:
 - Run with nsys cli:
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 - Nsight-systems setup on local workstation to use with Delta
 - sshfs mount example for linux box to Delta

Installation (Delta system, rgpu02 preliminary documentation)

For admins/sw team: Use Spack to install cuda, and the nsys command for Nsight Systems is included.

which nsys

```
[arnoldg@rgpu02 rgpu02]$ module load cuda
[arnoldg@rgpu02 rgpu02]$ which nsys
~/rgpu02/spack/opt/spack/linux-rhel8-zen/gcc-8.5.0/cuda-11.6.0-7ortdmqooz7ikzxpl4dvsqhqiflglvsa/bin/nsys
[arnoldg@rgpu02 rgpu02]$
```

Installation (NVIDIA Nsight Systems client on local desktop/laptop)

Open https://developer.nvidia.com/tools-overview and navigate to the <u>Developer Tools Downloads</u> button, then select <u>Nsight Systems</u> and your operating system. If you don't have an account at developer.nvidia.com set one up when prompted and when you have completed the forms, your download will begin. Install the application on your local machine. You will download output files from the server command line application and use the GUI locally on your laptop.

Run application on Delta

nsys with serial or python cuda code

```
$ srun nsys profile -o /path/to/mynysys.out --stats=true ./a.out
```

nsys wrapper for mpi and HPC cuda codes

```
[arnoldg@dt-login03 gromacs]$ cat nsys_wrap.sh
#!/bin/bash
# Use $PMI_RANK for MPICH, $OMPI_COMM_WORLD_RANK for openmpi, and $SLURM_PROCID with srun.
if [ $SLURM_PROCID -eq 1 ]; then
    nsys profile -e NSYS_MPI_STORE_TEAMS_PER_RANK=1 -o gmx.nsys --gpu-metrics-set=2 "$@"
else
    "$@"
fi
```



MPI rank example result (viewing with nsight on local desktop)

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	Top-Down View • Process [2091567] gmx_mpi (11 of 11 thread Filter 190,609 samples are used. Symbol Name • [Broken backtraces] spread_on_grid[gmx_pme_t const*, PmeAtomComm*, pmegrids_t gather f_bsplines[gmx_pme_t const*, float const*, bool, PmeAtom 36 unresolved fft5d_execute(fft5d_plan_t*, int, gmx_wallcycle*) ucp_worker_progress opal_timer_linux_get_cycles_sys_timer solve_pme_yzx[gmx_pme_t const*, t_complex*, float, bool, int, int) opal_progress ompi_coll_libhc_progress do_redist_pos_coeffs[gmx_pme_t*, t_commerc const*, bool, gmx:: void gmx:settleTemplate <gmx::simdfloat, 8,="" fl<br="" gmx::simdfbool,="">dd_pmeredist_figmx_pme_t*, PmeAtomComm*, gmx:ArrayRef<g n1fv_25</g </gmx::simdfloat,>	Self, % 13.87 9.45 4.46 3.61 3.46 3.13 2.97 2.67 1.83 1.67 1.51 1.25	Total, % 23.88 13.87 9.45 3.61 3.46 3.43 3.13 2.97 2.77 2.67 1.83 1.67 1.51 1.38 1.25	Module Name [Broken backtraces] /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /usr/lib64/us/lubuc_tb.so.0.0.0 /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /usr/lib64/libuct.so.0.0.0 /swispack/delta-2022-03/apps/openmpi/4.1.2-gcc-11.2.0-u2g3ure/lib64/libgromacs /usr/lib64/libucp.so.0.0.0.0 /swispack/delta-2022-03/apps/openmpi/4.1.2-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/openmpi/4.1.2-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/openmpi/4.1.2-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/openmpi/4.1.2-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs
	Top-Down View • Process [2091567] gmx_mpi (11 of 11 thread [*] Top-Down View • Process [2091567] gmx_mpi (11 of 11 thread • [Broken backtraces] spread_on_grid(gmx_pme_t const*, PmeAtomComm*, pmegrids_t gather_f_bsplines(gmx_pme_t const*, float const*, bool, PmeAtom 39 unresolved 7655_execute(fft5d_plan_t*, int, gmx_wallcycle*) ucp_worker_progress opal_timer_linux_get_cycles_sys_timer solve_pme_yzx(gmx_pme_t const*, t_complex*, float, bool, int, int) opal_progress do_redist_pos_coeffs(gmx_pme_t*, t_commrec const*, bool, gmx: void gmx:settleFemplate <gmx:simdfloat, 8,="" fl<br="" gmx::simdfbool,="">dd_pmeredist_f(gmx_pme_t*, PmeAtomComm*, gmx::ArrayRef<g n1fv_25 n2bv, 20</g </gmx:simdfloat,>	self, % - 13.87 9.45 4.46 3.61 3.51 1.28 1.24	Total, % 23.88 13.87 9.45 4.46 3.61 3.46 3.13 2.97 2.77 2.67 1.83 1.67 1.51 1.38 1.29 1.24	Module Name [Broken backtraces] [swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-202
	Top-Down View Process [2091567] gmx_mpi (11 of 11 thread Filter 190,609 samples are used. Symbol Name Isroad on grid(gmx_pme_t const*, PrneAtomComm*, prnegrids_t gather f_bsplines(gmx_pme_t const*, float const*, bool, PrneAtom 36 unresolved ff5d_execute(ff5d_plan_t*, int, gmx_wallcycle*) ucp_worker_progress opal_timer_linux_get_cycles_sys_timer solve_pme_yzx(gmx_pme_t const*, t_complex*, float, bool, int, int) opal_progress ompi_coll_libhccprogress do_redist_pos_coeffs(gmx_pme_t*, t_complex*, float, bool, int, int) opal_grogress do_redist_pos_coeffs(gmx_pme_t*, t_complex*, float, bool, gmx: void gmx:settleTemplate <gmx::simdfloat, <="" gmx::arrayref<g="" n1fv_25="" n2bv_20="" n2fv_20="" pre=""></gmx::simdfloat,>	Self, % - 13.87 9.45 4.46 3.13 2.97 2.67 1.83 1.67 1.51 1.38 1.25 1.24 1.16	Total, % 23.88 13.87 9.45 4.46 3.61 3.46 3.13 3.13 2.97 2.77 2.67 1.83 1.67 1.51 1.38 1.25 1.24 1.16	Module Name [Broken backtraces] /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /usr/lib64/lucx/libuct.so.0.0.0 /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /usr/lib64/libuct.so.0.0.0 /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftW3fs.o.3.6.10
	Top-Down View • Process [2091567] gmx_mpi (11 of 11 thread Filter 190.609 samples are used. Symbol Name • [Broken backtraces] spread_on_grid(gmx_pme_t const*, PmeAtomComm*, pmegrids_t gather f_bsplines(gmx_pme_t const*, float const*, bool, PmeAtom 36 unresolved fft5d_execute(fft5d_plan_t*, int, gmx_wallcycle*) ucp_worker_progress opal_timer_linux_get_cycles_sys_timer solve_pme_yzx(gmx_pme_t const*, t_complex*, float, bool, int, int) opal_progress do_redist_pos_coeffs(gmx_pme_t*, t_commerc const*, bool, gmx: void gmx:settleTemplate <gmx:simdfloat, 8,="" fl<br="" gmx:simdflool,="">dd_pmeredist_f(gmx_pme_t*, PmeAtomComm*, gmx::ArrayRef<g n1fv_25 n2bv_20 n2bv_25</g </gmx:simdfloat,>	Self, % - - - - - - - - - - - - -	Total, % 23.88 13.87 9.45 3.61 3.46 3.13 2.97 2.77 2.77 2.77 1.83 1.67 1.51 1.51 1.51 1.28 1.25 1.24 1.12	Module Name [Broken backtracs] /sw/spack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /usr/lib64/ucx/libuct.so.0.0.0 /sw/spack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /usr/lib64/libuct.so.0.0.0 /sw/spack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /usr/lib64/libucp.so.0.0.0 /sw/spack/delta-2022-03/apps/openmpi/4.1.2-gcc-11.2.0-u2g3ure/lib64/libgromacs /sw/spack/delta-2022-03/apps/openmpi/4.1.2-gcc-11.2.0-u2g3ure/lib64/libgromacs /sw/spack/delta-2022-03/apps/openmpi/4.1.2-gcc-11.2.0-u2g3ure/lib64/libgromacs /sw/spack/delta-2022-03/apps/openmpi/4.1.2-gcc-11.2.0-u2g3ure/lib64/libgromacs /sw/spack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /sw/spack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /sw/spack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /sw/spack/delta-2022-03/apps/ftm/3.3.10-gcc-12.0-aveixiu/lib/libftW3fs.o.3.6.10 /sw/spack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftW3fs.o.3.6.10 /sw/spack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftW3fs.o.3.6.10
	Top-Down View * Process [2091567] gmx_mpi (11 of 11 thread Top-Down View * Process [2091567] gmx_mpi (11 of 11 thread Filter 190,609 samples are used. Symbol Name * * [Broken backtraces] spread_on_grid(gmx_pme_t const*, PmeAtomComm*, pmegrids_t gather_f_bsplines(gmx_pme_t const*, float const*, bool, PmeAtom 39 unresolved #f15d_execute(fft5d_plan_t*, int, gmx_wallcycle*) ucp_worker_progress opal_timer_linux_get_cycles_sys_timer solve_pme_yzx(gmx_pme_t const*, t_complex*, float, bool, int, int) opal_progress odredist_pos_coeffs(gmx_pme_t*, t_complex*, float, bool, gmx: void gmx:settleftemplate <gmx::simdfloat, 8,="" fl<br="" gmx:simdfloot,="">void gmx:settleftemplate<gmx::simdfloat, gmx::arrayref<g<br="">n1fv_25 n2bv_20 n2fv_20 n1bv_25 +_start</gmx::simdfloat,></gmx::simdfloat,>	self, % 13.87 9.45 4.46 3.61 3.13 2.97 2.67 1.83 1.67 1.51 1.38 1.25 1.24 1.16 1.12	Total, % 23.88 13.87 9.45 4.46 3.61 3.46 3.13 2.97 2.67 1.83 1.67 1.51 1.51 1.38 1.25 1.24 1.16 1.12 0.96	Module Name [Broken backtraces] /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftW3fs.o.3.6.10 /swispack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftW3fs.o.3.6.10 /swispack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftW3fs.o.3.6.10 /swispack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftW3fs.o.3.6.10
	<pre></pre>	Self, % · 13.87 9.45 4.46 3.41 3.45 3.43 2.97 2.67 1.83 1.27 1.67 1.51 1.38 1.25 1.24 1.16 1.12 · 0.86	Total, % 23.88 13.87 9.45 4.46 3.61 3.43 2.97 2.77 2.67 1.83 1.67 1.51 1.25 1.24 1.12 1.25 1.24 1.12 0.96 0.86	Module Name [Broken backtraces] /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /usr/lib64/libuct.so.0.0.0 /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swispack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftw3fs.o.3.6.10 /swispack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftw3fs.o.3.6.10 /swispack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftw3fs.o.3.6.10 /swispack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftw3fs.o.3.6.10 /swispack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftw3fs.o.3.6.10 /swispack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftw3fs.o.3.6.10 /swispack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftw3fs.o.3.6.10 /swispack/delta-2022-03/apps/fttw/3.3.10-gcc-11.2.0-aveixiu/lib/libftw3fs.o.3.6.10
	<pre></pre>	self, % - 13.87 9.45 4.46 3.61 3.46 3.46 3.46 3.46 3.46 3.46 3.46 3.46 3.46 3.46 3.46 3.46 3.46 1.51 1.51 1.38 1.22 1.24	Total, % 23.88 13.87 9.45 4.46 3.61 3.13 2.97 2.77 2.67 1.83 1.67 1.51 1.38 1.24 1.16 1.12 1.24 1.16 0.96 0.86 0.76	Module Name [Broken backtraces] [Swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/ftw/3.3.10-gcc-11.2.0-aveixiu/lib/libftw3fs.o.3.6.10 /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/ftw/3.3.10-gcc-11.2.0-aveixiu/lib/libftw3fs.o.3.6.10 /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs /swlspack/delta-2022-03/apps/gromacs/2022.3-gcc-11.2.0-u2g3ure/lib64/libgromacs



Copy resultant files to your local laptop (Downloads/ or Documents/)

scp is shown below, you could also use globus online, sftp, or an sshfs mount from your laptop.

nsys output file example names

```
# Delta
[arnoldg@rgpu02 rgpu02]$ ls /tmp/nsys*
/tmp/nsys-report-988d.sqlite /tmp/nsys-report-b26d.nsys-rep
[arnoldg@rgpu02 rgpu02]$
# local laptop (MacOS example)
(base) galen@macbookair-m1-042020 ~ % cd Downloads
(base) galen@macbookair-m1-042020 Downloads % pwd
/Users/galen/Downloads
(base) galen@macbookair-m1-042020 Downloads % sftp arnoldg@rgpu02.delta.ncsa.illinois.edu
NCSA Delta System
Login with NCSA Kerberos + Duo multi-factor.
DUO Documentation: https://go.ncsa.illinois.edu/2fa
(arnoldg@rgpu02.delta.ncsa.illinois.edu) Password:
(arnoldg@rgpu02.delta.ncsa.illinois.edu) Duo two-factor login for arnoldg
Enter a passcode or select one of the following options:
1. Duo Push to XXX-XXX-1120
2. Duo Push to Ipad mini (iOS)
3. Duo Push to red ipod (iOS)
Passcode or option (1-3): 1
Connected to rgpu02.delta.ncsa.illinois.edu.
sftp> cd /tmp
sftp> mget nsys*
Fetching /tmp/nsys-report-988d.sqlite to nsys-report-988d.sqlite
/tmp/nsys-report-988d.sqlite
                                          100% 748KB 2.7MB/s 00:00
Fetching /tmp/nsys-report-b26d.nsys-rep to nsys-report-b26d.nsys-rep
/tmp/nsys-report-b26d.nsys-rep
                                            100% 288KB 1.7MB/s 00:00
sftp>
```

Open NVIDIA Nsight Systems

Under the File menu, select "open" then navigate to your Downloads/ folder and select the nsys* file of interest (nays-report-b26d.nsys-rep in this example). Explore the data in the GUI application.



File View Tools Help	성명 성명 영명 성명 영명 성명	
Project Explorer ×	Project 1 x nsys-report-b26	8d ×
Project 1 nsys-report-b26d	Analysis Summary reason	·
	Imported from /tmp/n	nsys-report-b1fe.qdstrm
	Import host rgpu0: computer	12. della nosa illinois edu
	CLI command /u/arm used x64/ns	oldg/gpu02/spack/opt/spack/linux-thel8-zen/goc-8.5.0/cuda-11.6.0-7ortdmqooz7/kzxpl4dvsqhqillg/vsa/hsight-systems-2021.5.2/target-linux- isys profile -o /tmp/mm.nsys.datstats=true /matr/dMul
	Show report file in folder	
	rgpu02.delta.ncsa	a.illinois.edu (0:0)
	Target	
	Local time at t=0	2022-01-27T11:20:18.882-06:00
	UTC time at t=0	2022-01-27T17:20:18.882Z
	TSC value at t=0	3785030664627213
	Platform	Linux
	OS	Red Hat Enterprise Linux 8.4 (Ootpa)
	Hardware platform	x86_64
	Serial number	Local (CLI)
	CPU description	AMD EPYC 7413 24-Core Processor
	GPU descriptions	NVIDIA A 100-55XM 400B NVIDIA A 100-55XM 400B NVIDIA A 100-55XM 400B NVIDIA A 100-55XM 400B
	NVIDIA driver version	495.29.05
	CPU context switch	supported
	GPU context switch	supported
		φ.



Python with NVTX

Install:

```
installing nvtx via pip
```

```
[arnoldg@rgpu02 nvtx]$ module load python cuda
[arnoldg@rgpu02 nvtx]$ C_INCLUDE_PATH=$CUDA_HOME/include pip install nvtx
Collecting nvtx
 Using cached nvtx-0.2.3.tar.gz (10 kB)
 Installing build dependencies ... done
 Getting requirements to build wheel ... done
 Preparing metadata (pyproject.toml) ... done
Building wheels for collected packages: nvtx
 Building wheel for nvtx (pyproject.toml) ... done
 Created wheel for nvtx: filename=nvtx-0.2.3-cp39-cp39-linux_x86_64.whl size=177533
sha256=875e0f9d4322d07db4bce397b4281ce301f348cf72e00629b0d7bc23a7db0231
 Stored in directory: /u/arnoldg/.cache/pip/wheels/66/7a/44/68c48f02433263010768b540b0e90bf5a224dd7e6612d88887
Successfully built nvtx
Installing collected packages: nvtx
Successfully installed nvtx-0.2.3
[arnoldg@rgpu02 nvtx]$
```

Run with nsys cli:

sample nsys run with stdout [arnoldg@rgpu02 nvtx]\$ nsys profile -o nvtx_simple.profile --stats=true ./nvtx_simple.py Warning: LBR backtrace method is not supported on this platform. DWARF backtrace method will be used. 0 1 2 3 4 Failed to create '/u/arnoldg/rgpu02/cuda/nvtx/nvtx_simple.profile.nsys-rep': File exists. Use `--force-overwrite true` to overwrite existing files. Generating '/tmp/nsys-report-1c93.qdstrm' Failed to create '/u/arnoldg/rgpu02/cuda/nvtx/nvtx_simple.profile.sqlite': File exists. Use `--force-overwrite true` to overwrite existing files. SKIPPED: /tmp/nsys-report-e498.sqlite does not contain CUDA trace data. SKIPPED: /tmp/nsys-report-e498.sqlite does not contain CUDA kernel data. SKIPPED: /tmp/nsys-report-e498.sqlite does not contain GPU memory data. SKIPPED: /tmp/nsys-report-e498.sqlite does not contain GPU memory data. [3/8] Executing 'nvtxsum' stats report NVTX Range Statistics: Time (%) Total Time (ns) Instances Med (ns) Min (ns) Avg (ns) Max (ns) StdDev (ns) Style Range _____ 50.0 10,010,633,188 1 10,010,633,188.0 10,010,633,188.0 10,010,633,188 10,010,633,188 0.0 PushPop f() 50.0 10,010,401,574 5 2,002,080,314.8 2,002,090,885.0 15,729 4,004,111,558 1,582,756,979.0 PushPop loop [4/8] Executing 'osrtsum' stats report Operating System Runtime API Statistics: Med (ns) Time (%) Total Time (ns) Num Calls Avg (ns) Min (ns) Max (ns) StdDev Name (ns) _____ _____ _____ 100.0 10,010,198,683 5 2,002,039,736.6 2,002,047,874.0 3,025 4,004,056,124 1,582,740,553.2 select 0.0 1,005,734 46 21,863.8 21,656.0 18,866 27,070 1,608.1 open64 495,879 49 10,120.0 4,960.0 1,262 67,747 0.0 12,669.1 read 38,843 10 3,884.3 3,957.5 3,186 4,559 0.0 408.1 mmap64 0.0 34,164 1 34,164.0 34,164.0 34,164 34,164 0.0 write 0.0 27,391 4 6,847.8 4,182.5 2,655 16,371 6,410.6 fopen64 3 2,200.7 1,232.0 6.602 1,172 0.0 4,198 1,730.0 pthread_cond_signal 0.0 3,647 1 3,647.0 3,647.0 3,647 3,647 0.0 sigaction 2,013 1 2,013.0 2,013 0.0 2,013.0 2,013 0.0 fread 1,923 1 1,923.0 1,923.0 1,923 0.0 1,923 0.0 fclose 0.0 1,472 1 1,472.0 1,472.0 1,472 1,472 0.0 fflush

[5/8]	Executing	'cudaapisum'	stats	report
-------	-----------	--------------	-------	--------

[6/8] Executing 'gpukernsum' stats report

[7/8] Executing 'gpumemtimesum' stats report

Delta script and nsight-systems view of the resulting report

```
#!/bin/bash
#SBATCH --job-name="numba_profile"
#SBATCH --partition=gpuA100x4-interactive
#SBATCH --mem=16G
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=2
                            # spread out to use 1 core per numa
#SBATCH --constraint="projects"
#SBATCH --gpus-per-node=1
#SBATCH --gpu-bind=closest # select a cpu close to gpu on pci bus topology
#SBATCH --account=bbka-delta-gpu
#SBATCH -t 00:10:00
cd $SLURM_SUBMIT_DIR
module load anaconda3_gpu
dcgmi profile --pause
srun nsys profile \
  --gpu-metrics-device=all \setminus
  ./nvtx-numba-jit.py
srun ncu \setminus
  --metrics "regex:.*" \setminus
  --target-processes all \setminus
  ./nvtx-numba-jit.py
dcgmi profile --resume
```

(Transferred the report1.nsys-rep back to local system using Globus Online , sftp \dots)



Nsight-systems setup on local workstation to use with Delta

Login to: https://developer.nvidia.com/nsight-systems (make an account if you need to), and download the client for your MacOS, Windows, or Linux local system.

You can use Globus Online, rsync, sftp, or sshfs (linux) to transfer files (or view files as local filesystem mounts in the case of sshfs) with the local nsightsystems client.

sshfs mount example for linux box to Delta

sshfs example mounting delta projects

```
galen@galen-HP-ProBook-455-G6:~$ sshfs arnoldg@dt-login03.delta.ncsa.illinois.edu:/projects/bbka delta_projects/
arnoldg@dt-login03.delta.ncsa.illinois.edu's password:
(arnoldg@dt-login03.delta.ncsa.illinois.edu) Duo two-factor login for arnoldg
Enter a passcode or select one of the following options:
1. Duo Push to XXX-XXX-1120
2. Duo Push to Ipad mini (iOS)
3. Duo Push to red ipod (iOS)
4. Duo Push to red ipod (iOS)
4. Duo Push to Android
Passcode or option (1-4): 115489
galen@galen-HP-ProBook-455-G6:~$ df -h delta_projects/
Filesystem Size Used Avail Use% Mounted on
arnoldg@dt-login03.delta.ncsa.illinois.edu:/projects/bbka 1000T 60T 941T 6% /home/galen/delta_projects
```

Launch nsight-systems and define a target under the default opening view. Even if you cannot get nsight-systems to ssh to the target, you need to define it so that nsight-systems will present you with the .nsys-rep file type when you try to open a profile from delta that was transferred to local via GO/sftp/rsync or viewable via the sshfs fuse mount like shown above:

	NVIDIA Nsight Systems 2022.4.1			
<u>F</u> ile <u>V</u> iew <u>T</u> ools <u>H</u> elp				
Project Explorer ×	Project 2 × report1 ×			
Froject 2	 arnoldg@dt-login03.delta.ncsa.illinois.e Communication error More info Last used target: arnoldg@dt-login03.delta.ncsa.illinois.edu (SSH). Select Select a target to see available options. 			

Then open the profile report generated from an srun nsys ... at Delta. (navigate to Download or the live sshfs fuse mount)

View Tools Help			NVIDIA N	sight Systems 2022.4.1			- 0
oject Explorer	×	Project 2 × report1 ×					
Project 2		≡ Timeline View →			Ξ Θ	1x	() 2 errors, 4 warnings, 17 messa
Teporti		•	0s	10s	20s	30s	40s
		▶ CPU (64)					
		CUDA HW (0000:07:00.0 - NVI					
		▼ Threads (11)					
		 [3075328] python3 - 				, <u>marina</u> malana	
		OS runtime libraries	i initia i i Initia i initia i		i hadaa ma	The state of the s	աստաստանությունը Հայաստանությունը Հայաստանությունը
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Proceed to use nsight-systems. A stats view of the GPU Summary is shown. This is usually a good performance analysis starting point showing utilization of kernels vs times to transfer data between the host computer and the gpu accelerator.



https://docs.nvidia.com/cuda/cuda-c-programming-guide

User Guide :: Nsight Systems Documentation (nvidia.com) (nsys higher level and cuda api)

Nsight Compute CLI :: Nsight Compute Documentation (nvidia.com) (ncu lower level and counters)

GitHub - quasiben/nvtx-examples (sample python test codes)