TRAVERSE GPU Version

How to download:

$ git clone -b traverse-gpu https://github.com/PrincetonUniversity/M3DC1.git ./M3DC1

How to compile:

$ cd M3DC1/unstructured
$ module load nvhpc/21.5
$ export PATH=/projects/M3DC1/bin:/projects/M3DC1/openmpi/traverse-nvidia/bin:$PATH

For CPU version:
$ make ARCH=traverse_gpu COM=1 OPT=1
or
$ make ARCH=traverse_gpu 3D=1 OPT=1

For GPU version:
$ make ARCH=traverse_gpu COM=1 OPT=1 ACC=1
or
$ make ARCH=traverse_gpu 3D=1 OPT=1 ACC=1

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How to run:
Right now it is better to use mpirun with a hostfile to run on traverse.

```
$ export PATH=/projects/M3DC1/bin:/projects/M3DC1/openmpi/traverse-nvidia/bin:$PATH
$ gethostfile
$ mpirun -np 32 -hostfile hostfile --bind-to none ./m3dc1_2d_complex
-ksp_type preonly -pc_type lu -pc_factor_mat_solver_type mumps
-mat_mumps_icntl_23 5000 -ksp_converged_reason
-ksp_error_if_not_converged true -on_error_abort
```

or

```
$ mpirun -np 128 --hostfile hostfile --bind-to none ./m3dc1_3d
-options_file options_bjacobi
```

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Here is an example of batch file

```
#!/bin/bash
#SBATCH --job-name=m3dc1
#SBATCH -N 4
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=128
#SBATCH --gpus-per-node=4
#SBATCH --time=6:00:00
#SBATCH --output=/dev/null
#SBATCH --error=/dev/null
```

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```
exec 1<>"output.$SLURM_JOB_ID"
exec 2>&1

module load nvhpc/21.5

export
PATH=/projects/M3DC1/bin:/projects/M3DC1/openmpi/tra
verse-nvidia/bin:$PATH
gethostfile

command="mpirun -np 128 --hostfile hostfile --bind-to
none ./m3dc1_3d
-options_file options_bjacobi"
echo $command
eval $command
```

I also compiled a working split_smb file and put it at /projects/M3DC1/bin