nekRS log

Introduction:

This document includes all the details and steps needed to run the nekRS turbPipePeriodic case. The case is for a periodic smooth pipe turbulent flow at a frictional Reynolds number of 550.

https://github.com/Nek5000/nekRS/tree/master/examples/turbPipePeriodic

The simulations were run on MASC, a research computer with GPUs: https://masc-portal.soe.manchester.ac.uk/website/content/documentation/userguide/

Steps were taken on an ssh terminal.

How to compile nekRS:

clone repo

```
git clone https://github.com/Nek5000/nekRS.git
```

load modules

```
module load gcc/13.2.0
module load cuda/11.8.0
module load cmake/3.27.9
module load openmpi/5.0.3
```

those depend on machine

run: `module avail <keyword>` to find available modules

build and install (under nekRS main directory)

```
CC=mpicc CXX=mpic++ FC=mpif77 ./nrsconfig [-
DCMAKE_INSTALL_PREFIX=$HOME/.local/nekrs]
```

(took 2 minutes approx.)

```
-- Installing: /mnt/iusers01/fse-ugpgt01/mace01/t62601ej/.local/nekrs/include/solvers/cvode/cvode.hpp
-- Installing: /mnt/iusers01/fse-ugpgt01/mace01/t62601ej/.local/nekrs/include/pointInterpolation
-- Installing: /mnt/iusers01/fse-ugpgt01/mace01/t62601ej/.local/nekrs/include/pointInterpolation/pointInterpolation.hpp
-- Installing: /mnt/iusers01/fse-ugpgt01/mace01/t62601ej/.local/nekrs/include/udf
-- Installing: /mnt/iusers01/fse-ugpgt01/mace01/t62601ej/.local/nekrs/include/udf/udf.hpp
-- Installing: /mnt/iusers01/fse-ugpgt01/mace01/t62601ej/.local/nekrs/include/nrs.hpp
-- Installing: /mnt/iusers01/fse-ugpgt01/mace01/t62601ej/.local/nekrs/udf/CMakeLists.txt
-- Installing: /mnt/iusers01/fse-ugpgt01/mace01/t62601ej/.local/nekrs/nekInterface
-- Installing: /mnt/iusers01/fse-ugpgt01/mace01/t62601ej/.local/nekrs/nekInterface/Makefile
-- Installing: /mnt/iusers01/fse-ugpgt01/mace01/t62601ej/.local/nekrs/nekInterface/nekInterface.f
-- Installing: /mnt/iusers01/fse-ugpgt01/mace01/t62601ej/.local/nekrs/nekInterface/NEKINTF
-- Installing: /mnt/iusers01/fse-ugpgt01/mace01/t62601ej/.local/nekrs/doc/parHelp.txt

Hooray! You're all set. The installation is complete.
```

export to bashrc or bash_profile:

```
echo 'export NEKRS_HOME=$HOME/.local/nekrs' >> ~/.bashrc
echo 'export PATH=$NEKRS_HOME/bin:$PATH' >> ~/.bashrc
```

Changes in scripts:

modify turbPipe.geo:

```
// GRID SETTINGS ////////////////////////////////////

// Geometrical parameters
// Note: r<RB<R
R=0.1;   //Pipe radius
r=0.7;
RB=0.978343;
lambda=0.3;   //=R_{arc}/R
Lz=6;   //length in z-dir

// Grid Paramaters
Nc=12;   // no. of nodes (=#elem+1) in azimuthal direction
NB=2;   // no. of elemtns adjacent to the wall
NM=6;   // no. of nodes (=#elem+1) between the near wall layer and central square part

compressRatio_B=0.85;  //ratio of grid compression toward the wall (<1)
compressRatio_M=0.87;  //compression ratio in the middle layer
Nz=20;  //no of elements in z-dir (streamwise)

////////////////////////////////////////////////
```

download gmsh module:

```
module avail gmsh
module load gmsh/4.12.2
```

generate mesh:

```
gmsh turbPipe.geo -3 -order 2
```

gmsh2nek has to be built separately from Nek5000 or KTH-Framework (older gmsh2nek) repo

```
git clone https://github.com/Nek5000/Nek5000.git
cd Nek5000/tools
./maketools all
```

run gmsh2nek: ~/Nek5000/bin/gmsh2nek
/home/t62601ej/KTH_Framework/Nek5000/bin/gmsh2nek (run this from KTH-Framework)

run genmap: ~/Nek5000/bin/genmap (or from KTH framework)

in turbPipe.par:

change viscosity to `viscosity = -2650` (to match Re_tau=180 case)

change `boundaryTypeMap = periodic, periodic, wall`

no other changes required at this stage

time-stepping, viscosity (and therefore frictional viscosity) are set in turbPipe.par
mesh is fixed in turbPipe.geo

Write batch file:

batch file is written in SLURM to submit job in accordance to the MASC documentation

find batch file turbPipe.sh below:

```
#!/bin/bash
#SBATCH --job-name=turbPipe
#SBATCH --output=turbPipe.out
#SBATCH --ntasks=1
#SBATCH --gres=gpu:1
#SBATCH --time=02:00:00
#SBATCH --partition=debug

module load cuda/11.8.0
module load openmpi/5.0.3
module load cmake/3.27.9

# Point to local NekRS install
export NEKRS_HOME=$HOME/.local/nekrs
export PATH=$NEKRS_HOME/bin:$PATH

# build
nekrs --setup turbPipe.par

# run
mpirun -np 1 nekrs turbPipe
```

Visualise results:

tail turbPipe.out and squeue to monitor results

runtime statistics can be obtained and analysed from end of turbPipe.out

results can be obtained by visualising turbPipe.nek5000 from the directory (visnek seems to be integrated into nekRS)

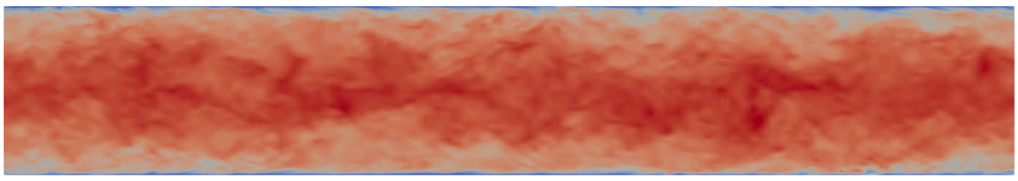

Figure 1: default case (no change) from turbPipePeriodic in nekRS repo