# Running on Rocket

## Logging into Rocket

In order to check if you have access to Newcastle University’s Rocket cluster try to login at rocket.hpc.ncl.ac.uk using a ssh client:

* Linux – use the following command on a terminal

$ ssh <user>@rocket.hpc.ncl.ac.uk

* Windows – download and install PuTTY. Open the application and set <user>@rocket.hpc.ncl.ac.uk in the “Host Name” input field. Press the “Open” button.

Note that <user> must be your Newcastle University user name.

If you are able to connect to rocket login node you are already subscribed as a NUFEB project user. If not, you will need to request access to Ben Allen

## Downloading NUFEB source code

Use the following command to download the NUFEB source code from GitHub:

$ git clone –recursive <https://github.com/shelllbw/nufeb.git>

This will create a new nufeb folder. You will need an active user at GitHub and the permission to access the source code. If your access is denied please contact Bowen Li.

## Compiling the code with Intel compiler

Once you have download the source code use the following command to compile (assuming that you have just cloned the repository):

$ cd nufeb

$ tar –xvzf libvtk\_rocket.tar.gz –C $HOME

$ cd code/lammps5Nov16/src

$ module load intel

$ make yes-granular

$ cp ../lib/vtk/Makefile.lammps.rocket ../lib/vtk/Makefile.lammps

$ make yes-user-vtk

$ make yes-user-nufeb

$ make –j8 rocket\_intel

The first command change the current directory to the previously created nufeb folder during the git clone command. The second command will extract the VTK library files to your home directory. This is required if you want to visualize the simulation using Paraview, using dump custom/vtk or dump grid commands. The third command changes the current directory to the LAMMPS source folder. The forth command loads the intel compiler environment on Rocket. The fifth command includes the GRANULAR package in the compilation, which is required for the Hookean and Hertzian contact forces used for the mechanical model. The sixth and seventh commands selects the Makefile.lammps.rocket file as the compiling script for the USER-VTK package, and adds it to the build process, respectively. Again, they are only required if you want to visualize the result using Paraview. The eighth command includes the USER-NUFEB package for compilation. And finally, the last command starts the compilation process using 8 processes.

## Compiling the code with GNU compiler

Once you have download the source code use the following command to compile (assuming that you have just cloned the repository):

$ cd nufeb

$ tar –xvzf libvtk\_rocket.tar.gz –C $HOME

$ cd code/lammps5Nov16/src

$ module load GCC/6.4.0-2.28

$ module load OpenMPI/2.1.1-GCC-6.4.0-2.28

$ make yes-granular

$ cp ../lib/vtk/Makefile.lammps.rocket ../lib/vtk/Makefile.lammps

$ make yes-user-vtk

$ make yes-user-nufeb

$ make –j8 rocket\_gnu

The first command change the current directory to the previously created nufeb folder during the git clone command. The second command will extract the VTK library files to your home directory. This is required if you want to visualize the simulation using Paraview, using dump custom/vtk or dump grid commands. The third command changes the current directory to the LAMMPS source folder. The forth command loads the GCC compiler environment on Rocket. The fifth command loads the OpenMPI environment on Rocket. The sixth command includes the GRANULAR package in the compilation, which is required for the Hookean and Hertzian contact forces used for the mechanical model. The seventh and eighth commands selects the Makefile.lammps.rocket file as the compiling script for the USER-VTK package, and adds it to the build process, respectively. Again, they are only required if you want to visualize the result using Paraview. The ninth command includes the USER-NUFEB package for compilation. And finally, the last command starts the compilation process using 8 processes.

## Running a simulation

To run a job on Rocket it must be submitted to SLURM, that manages all job queues, priorities and computation nodes distribution. SLURM expects a job script as input, containing all the information needed for the execution. A job script example is given below, depending on which compiler was used:

* Intel compiler

#!/bin/bash

#SBATCH -A tcnufeb

#SBATCH --ntasks=4

module load intel

export PATH=$PATH:$HOME/nufeb/code/lammps5Nov16/src

export LD\_LIBRARY\_PATH=$LD\_LIBRARY\_PATH:$HOME/local/lib

srun lmp\_rocket\_intel -in Inputscript.lammps

* GNU compiler

#!/bin/bash

#SBATCH -A tcnufeb

#SBATCH --ntasks=4

module load GCC/6.4.0-2.28

module load OpenMPI/2.1.1-GCC-6.4.0-2.28

export PATH=$PATH:$HOME/nufeb/code/lammps5Nov16/src

export LD\_LIBRARY\_PATH=$LD\_LIBRARY\_PATH:$HOME/local/lib

srun lmp\_rocket\_gnu -in Inputscript.lammps

The line “#SBATCH -A tcnufeb” is always required to set the job as part of the NUFEB project. The “--ntasks” option sets the number of processes to run the simulation. This has to be in accordance to the processors command in Inputscript.lammps.

Considering that you job script file name is “job” and is located in the same folder as the Inputscript.lammps file, run the following command to submit the job:

$ sbatch job

You can check the status of your job at any time, by using the following command:

$ squeue –u <user>

Please read the Rocket on-line documentation for further information (<http://www.ncl.ac.uk/itservice/research/hpc/hpcquick-startguide/>).