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Computer Science in Ocean and Climate Research

Exercise 8

Tutorial: (Exercise June 2nd + 9th, 2020) and **Home** (until June 16th, 2020):
Topic of this exercise is the usage of a given climate model on the CAU High Performance Computer system. The model and software that we use is described in the lecture on Monday, May 25th.

1. We use the NEC-HPC Linux cluster of Kiel University.

   - Form groups of two students. The username and preliminary password for each group you will obtain in the tutorial on June, 2nd.
   - From a computer outside the university network, you need to log in to the HPC system via Virtual Private Network (VPN). The account that you got includes an access to the university network via VPN. Follow the instructions to install a VPN client on the University Computing Centre's webpage `www.rz.uni-kiel.de`.
   - Find out how to log in to the NEC-HPC Linux cluster on the webpage of the University Computing Centre.

2. We use the software Metos3D (The Marine Ecosystem Toolkit for Simulation and Optimization in 3D).

   - Follow the instructions on `https://metos3d.github.io` and install the software on your account on the NEC-HPC cluster.
   - We need the Simulation, Model and Data packages. In which directory has the software been installed?
   - Add the Metos3D path to your `PATH` shell variable in the `.bashrc` file as displayed during the installation.
   - To compile, we need three software packages
     - C/Fortran compiler
     - MPI compiler (parallel computing)
     - PETSc library

     that have to be loaded:

     ```
     module load intel17.0.4 intelmpi17.0.4 petsc3.7.6intel
     ```

   - Compile the simulation package with the N-DOP model as exemplary model:

     ```
     metos3d simpack N-DOP
     ```

     This will generate an executable named `metos3d-simpack-N-DOP.exe`.
   - If you run the executable with

     ```
     ./metos3d-simpack-N-DOP.exe
     ```

     it will ask for an option file to set up the simulation parameters.

- In the model directory, here

  `.metos3d/model/model/N-DOP/option`

  you find one file `test.N-DOP.option.txt` that defines a short test run.
- Perform this test run with:

  `./metos3d-simpack-N-DOP.exe model/N-DOP/option/test.N-DOP.option.txt`
- Look in the options file what is defined there. A `#` at the beginning of the line marks a comment.

3. To run a longer simulation, you have to start a batch job.

   - This is done by writing a batch script file

     ```
     #!/bin/bash
     #PBS -T intmpi
     #PBS -b 1
     #PBS -l cpunum_job=16
     #PBS -l elapstim_req=02:00:00
     #PBS -l memsz_job=10gb
     #PBS -N test-N-DOP
     #PBS -o test-N-DOP.out
     #PBS -j o
     #PBS -q clexpress
     cd $PBS_O_WORKDIR
     module load intel17.0.4 intelmpi17.0.4 petsc3.7.6intel
     mpirun $NQSII_MPIOPTS -np 16 ./metos3d-simpack-N-DOP.exe option-file.txt
     qstat -f ${PBS_JOBID/0:}
     ```
   - You find this example script (`nec-script.sh`) in the OLAT exercise folder.
   - It can be copied to your NEC account using the `scp` command.
   - Look on the Computing Centre webpage to understand what is defined in this file.
   - Modify the option file to set up a longer simulation. Change the following lines:

     ```
     -Metos3DMatrixCount                          12
     -Metos3DTimeStepCount                      2880
     -Metos3DSpinupCount                         100
     ```

     The last of these three options defines the number of model years to be simulated. As mentioned in the lecture, usually 3'000 model years are necsessary to obtain a steady solution.
   - Submit the batch script using the `qsub` command.
   - In the options file, also the location and the names of the output files are defined:

     ```
     -Metos3DTracerOutputDirectory              work/
     -Metos3DTracerOutputFile                   N.petsc,DOP.petsc
     ```
   - With the `qstat` command, you can check the status of your job. If it is finished, check if the above files are generated.