ASPECT installation on ARCHER2

Special thanks to William Lucas and the ARCHER2 service desk for helping create this guide.

Guide last updated 20/03/2024, installing ASPECT ver. 2.6-pre.

All writing in red relates to a bug currently on ARCHER2 so may not be necessary steps later on. Extract from an email from William Lucas about the bug:

Given the errors you're seeing, I'm reminded of an issue I helped another user with last year. deal.II and ASPECT both contain some definitions which among them include overloaded functions which return MPI_CXX_BOOL for bool types. The problem is that in Cray MPICH, the MPI installation provided as part of ARCHER2's programming environment, MPI_CXX_BOOL is mapped to MPI_TYPE_NULL. ASPECT uses this header and attempts to broadcast bools, but this resolves as MPI trying to broadcast MPI_TYPE_NULL, which fails.

I was informed by HPE that they are tracking this bug and it will be fixed, but until that fix is made and installed on ARCHER2 it unfortunately necessitates a couple of changes to the deal.II and ASPECT code.

Installing deal ii

Create a directory to store candi and ASPECT into. Here I named the directory dw as a way of keeping things clean:

mkdir dw

cd dw

mkdir aspect

Create a copy of the candi Git repository:

git clone https://github.com/dealii/candi

Move into the cray platform file and then change the packages to install SUNDIALS if necessary:

cd candi/deal.II-toolchain/platforms/contributed

nano cray.platform

Replace the last line:

-D MPI_CXX_LIBRARIES=\"${MPICH_DIR}/lib/libmpichcxx.so;${MPICH_DIR}/lib/libmpich.so\" "

With:

-D MPI_CXX_LIBRARIES=\"${MPICH_DIR}/lib/libmpich.so\" "

Also to install SUNDIALS replace the line:

PACKAGES="load:dealii-prepare once:cmake once:p4est once:trilinos once:parmetis once:petsc dealii"

With:

PACKAGES="load:dealii-prepare once:cmake once:p4est once:sundials once:trilinos once:parmetis once:petsc dealii"

Move back into the candi directory:

cd ../../../

Setup the environment to make sure the following compiler wrappers will be used:

module load PrgEnv-gnu cray-libsci

module unload atp

export CRAYPE_LINK_TYPE=dynamic

export CC=cc

export CXX=CC

export FC=ftn

export FF=ftn

Run candi to install dealii and other libraries, this will take a while (>1 hour). Here /work/n03/n03/llongley/dw/aspect refers to where I'm installing dealii so you will have to change this to your own personal directory. -j 8 refers to the number of processors used:

./candi.sh --prefix=/work/n03/n03/llongley/dw/aspect -j 8 --platform=./deal.II-toolchain/platforms/contributed/cray.platform

Replace line following wills instructions:

cd ../

cd aspect/deal.II-v9.5.1/include/deal.II/base

nano mpi.h

Search and replace the line return MPI_CXX_BOOL; with return MPI_C_BOOL;

Installing ASPECT

Create a new directory to install ASPECT into. Here I named it aspect-2.5.0 as it's the most recent version:

cd ../../../../

cd aspect

mkdir aspect-2.5.0

Move out of the directory and clone the ASPECT source code:

cd ../../

git clone https://github.com/geodynamics/aspect.git (for most recent version)

git clone -b aspect-2.5 https://github.com/geodynamics/aspect.git (for version 2.5.0)

Go into the ASPECT source directory, create a build directory, and move into it:

cd aspect

cd source

nano utilities.cc

Search for MPI_CXX_BOOL and replace:

```
inline MPI_Datatype
    mpi_type_id(const bool *)
    {
# if DEAL_II_MPI_VERSION_GTE(2, 2)
     return MPI_CXX_BOOL;
# else
     return MPI_C_BOOL;
# endif
    }
```

With:

```
inline MPI_Datatype
    mpi_type_id(const bool *)
    {
# if DEAL_II_MPI_VERSION_GTE(2, 2)
     return MPI_C_BOOL;
# else
```

return MPI_C_BOOL;

 # endif

}

cd *../*

mkdir build

cd build

Configure the build with cmake. Here we're specifying where dealii is installed and where ASPECT should be installed:

cmake .. -DDEAL_II_DIR=/work/n03/n03/llongley/dw/aspect/deal.II-v9.5.1 -DCMAKE_INSTALL_PREFIX=/work/n03/n03/llongley/dw/aspect/aspect-2.5.0

To run in optimised mode (if you're wanting to use debug mode then you can skip this step):

make release

Compile ASPECT. This takes a few minutes:

make -j 8

Install to the location specified by the -DCMAKE_INSTALL_PREFIX flag:

make install

The only potential issues should be if deal.II can't be found at the location provided to cmake, or if the install location isn't writable. Making sure deal.II has been installed to the correct location and that -DDEAL_II_DIR points to it should prevent the first problem; as long as -DCMAKE_INSTALL_PREFIX is in your own directories you should be ok on the second front.

Running ASPECT

ASPECT can be ran using:

sbatch slurm.sh

When slurm.sh is:

```
#!/bin/bash --login

#SBATCH --job-name=aspect2
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=128
#SBATCH --cpus-per-task=1
#SBATCH --time=00:20:00

# Replace [budget code] below with your project code (e.g. t01)
#SBATCH --account=n03-derby
#SBATCH --partition=standard
#SBATCH --qos=standard

# Recommended environment settings
# Stop unintentional multi-threading within software libraries
export OMP_NUM_THREADS=1
# Ensure the cpus-per-task option is propagated to srun commands
export SRUN_CPUS_PER_TASK=$SLURM_CPUS_PER_TASK

# load any modules you need
module dwap PrgEnv-cray PrgEnv-gnu
module load cray-libsci
module load cmake
module unload atp


# srun launches the parallel program based on the SBATCH options
srun --distribution=block:block --hint=nomultithread
/work/n03/n03/llongley/dw/aspect/aspect-2.5.0/bin/aspect aspect_parameter_file.prm
```