CP2K in the cloud

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This article describes how to deploy a Microsoft Azure compute instance to use with a CP2K compiled from scratch.

First, you need an instance. Login to [MS Azure](#) and switch to the resources tab. Select "Add" in the top menu to create a new virtual machine (or dedicated server if you go for the beefy machines). Select "Ubuntu Server" machines from Canonical. Select Ubuntu 16.04, one of the instance sizes matching your needs and fill all mandatory fields. For simple single-node calculations their actual content is of minimal interest. Make sure to paste your public SSH key into the appropriate field (the whole contents of the file *.ssh/id_rsa.pub* on most machines). As soon as your machine is available, you can directly login via SSH. Note that you specified the username during setup, so that username together with the IP/URL and your SSH key should allow you to connect directly. Depending on the availability provisioning your machine can take up to some 15 minutes.

Update the software database

```
sudo apt-get upgrade
```

Install the bare dependencies of CP2K and helpful tools:

```
sudo apt-get install build-essential gfortran libscalapack-mpi-dev \
libscalapack-openmpi1 libscalapack-pvm-dev libscalapack-pvm1 \
libfftw3-3 libfftw3-dev libblas-dev liblapack-dev libint-dev \
python checkinstall
```

Now two dependencies have to be built that are either not available in the repository or just compiled with the wrong flags.

```
cd
mkdir libxc
cd libxc
wget 'http://www.tddft.org/programs/octopus/down.php?file=libxc/libxc-2.2.3.tar.gz' -O 'libxc-2.2.3.tar.gz'
tar xzf libxc-2.2.3.tar.gz
cd libxc-2.2.3/
./configure
make -j XX
```

with XX in the last line being the number of cores your machine offers. Now libxc is compiled. To help easy uninstalling,

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