Install MCCE

Download and installation procedure

* [Download and Install MCCE](#)

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MCCE runs on Linux and Mac OSX natively.

On Windows, you will need a Linux environment. It could be a virtual box instance, Cygwin, or Linux subsystem that is included in Windows. Here is a short guide of installing Windows Subsystem Linux (to be done):

Prerequisites

Compilers:

C, gfortran

MCCE comes with two parts:

- MCCE main code in c/c++
- Poisson Boltzmann equation solver delphi in c/fortran

You need basic Linux program tools like make and ar utility. They usually some with the operating system. If not, install them. On Ubuntu, run

`sudo apt install build-essential`

It is recommended to use the compilers under conda. Conda provides compilers and other programming tools under user space. If you don't have conda, you can follow instruction here

https://docs.conda.io/en/latest/miniconda.html to install miniconda.

Python and modules

We need Python3 and optionally these modules: numpy, scipy, matplotlib, pygraphviz, pandas, xlrd, and openpyxl

- Install Miniconda Python3: https://docs.conda.io/en/latest/miniconda.html
- After installing Miniconda, install these optional modules for data analysis:

```
conda install requests numpy scipy matplotlib pygraphviz pandas xlrd openpyxl multiprocess
```

To install gfortran compiler that is compatible for delphi:

Create mcce environment

```
conda create -n mcce
conda activate mcce
```

Install compilers

```
conda install -c conda-forge gcc gfortran
```

Now roll back gfortran to 9.5.0 (delphi requires an old compiler)

```
conda install -c conda-forge gfortran=9.5.0
```

Install MCCE

Download from github

Under a terminal window, run:

```
git clone https://github.com/GunnerLab/Stable-MCCE.git
```

Compile the code

The above command creates a directory named Stable-MCCE, enter the directory and compile:

```
$ cd Stable-MCCE
$ make clean
$ make
```

Configure environment

Find the path of Stable-MCCE installation directory:

```
(base) jmao@pc:~/projects/Stable-MCCE$ pwd
/home/jmao/projects/Stable-MCCE
```

In my case the installation directory is **/home/jmao/projects/Stable-MCCE/**

Add the executable to your path:

```
export PATH=/home/jmao/projects/Stable-MCCE/bin: $PATH
```

Remember to replace the installation directory **/home/jmao/projects/Stable-MCCE/** with your own installation path.

Also put this line at the end of .bashrc file under your home directory so that the environment is properly set every time you open a terminal window.