desorption

Release 0.0.0

Many

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CHAPTER

ONE

INSTALLATION AND RUNNING

1.1 Docker

Note: For use on supercomputers, use singularity instead

First, docker needs to be installed. Docker Desktop can be installed at https://docs.docker.com/get-docker/

```
docker pull dejac001/mcccs-mn
docker run -ti -v $PWD:/home/ dejac001/mcccs-mn # run interactively inside container
```

Then, the image can be accessed interactively by

```
docker run -ti -v $PWD:/home/ dejac001/mcccs-mn # run interactively inside container
```

1.2 Singularity

```
module load singularity
singularity pull docker://dejac001/mcccs-mn
```

Note: It is a good practice to move the singularity image, which is large, to a shared directory (e.g., `/home/<groupname>/shared/`)

The code can then be run using

```
module load singularity
cd ${workdir}  # change to working directory where input files are
singularity exec path/to/mcccs-mn_latest.sif topmon
```

where `path/to/mcccs-x_latest.sif` is the relative or absolute path to the singularity image made during installation.

To run with multiple processors (e.g. 2), the last line is be replaced with

```
singularity exec path/to/mcccs-mn_latest.sif mpirun -np 2 topmon
```

See also:

https://www.msi.umn.edu/sites/default/files/Singularity_Containers.pdf

1.3 Windows 10

On Windows 10, installing and running can be performed using Docker or Ubuntu. The instructions for Docker are given above. Otherwise, install Windows-Subsystem-for-Linux

then install Ubuntu from the App store and then follow the instructions below for Ubuntu.

1.4 Ubuntu

The dockerfiles and docker image is made in ubuntu, so the same commands can be made as those in the docker files.

First, the dependencies need to be installed. The associated dockerfile looks like the following

```
FROM ubuntu
MAINTAINER <dejac001@umn.edu>

RUN apt-get update
RUN DEBIAN_FRONTEND="noninteractive" \
   apt-get -y install gfortran cmake git mpi mpich
```

To install the ubuntu dependencies, type in the commands **after** `RUN`.

Second, the code needs to be cloned from the repository. The associated dockerfile looks like

```
FROM dejac001/mcccs-x-base
MAINTAINER <dejac001@umn.edu>

RUN cd /lib \
    && git clone https://github.com/dejac001/desorption.git MCCCS-MN \
    && mkdir -p MCCCS-MN/build && cd MCCCS-MN/build/ \
    && cmake -D CMAKE_BUILD_TYPE=RELEASE .. && make -j 2 \
    && ln -sf /lib/MCCCS-MN/build/src/topmon /usr/bin/topmon
```

Again, installation in ubuntu requires using the same commands **after** `RUN`.

1.5 Minnesota Supercomputing Institute

1.5.1 Mesabi

```
module load cmake
git clone https://github.com/dejac001/desorption.git MCCCS-MN
cd /path/to/MCCCS-MN
mkdir build && cd build/
cmake ..
make -j 2
```

Note: This uses the *GNU* 4.8.5 fortran compiler. You can try using other compilers too.

1.6 Siepmann Group

1.6.1 Metropolis

```
module purge
git clone https://github.com/dejac001/desorption.git MCCCS-MN && cd MCCCS-MN
module load cmake intel impi
mkdir build && cd build
FC=ifort cmake ..
make -j 2
```

CHAPTER

TWO

INPUT FILES

Note: See the following for restructured text (.rst) file formats https://docutils.sourceforge.io/docs/user/rst/quickref.html#definition-lists

2.1 fort.4

2.1.1 mc_shared

seed (integer) Random number seed, defaults to ??

nbox (integer) Number of boxes in simulation, defaults to ??

nmolty (integer) Number of molecule types in simulation, defaults to ??

2.1.2 analysis

2.1.3 mc_volume

2.1.4 mc_swatch

2.1.5 mc_swap

2.1.6 mc_cbmc

2.1.7 mc_simple

2.1.8 SIMULATION_BOX

2.1.9 MOLECULE_TYPE

2.1.10 MC_SWAP

2.1.11 MC_SWATCH

2.1.12 INTERMOLECULAR_EXCLUSION

2.1.13 UNIFORM_BIASING_POTENTIALS

2.2 topmon.inp

Holds many bead parameters

2.3 fort.77

Restart file

CHAPTER

THREE

ALGORITHMS

A mathematical equation can be written like

$$a + b = c^2$$

which is similar to latex

3.1 Coupled-Decoupled Configurational-Bias Monte Carlo

See reference [MS99]

3.2 CBMC

See references ??

3.3 SAFE-CBMC

3.4 AVBMC

CHAPTER

FOUR

REFERENCES

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INDICES AND TABLES

- genindex
- modindex
- search

BIBLIOGRAPHY

[MS99] M G Martin and J I Siepmann. Novel Configurational-bias Monte Carlo Method for Branched Molecules. Transferable Potentials for Phase Equilibria. 2. United-atom Description of Branched Alkanes. *J. Phys. Chem. B*, 103:4508–4517, 1999.