# The Experiments of Parallel Simulated Annealing on Lennard Jones Problem

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# PSA Settings

## Sequential Simulated Annealing

**Objective Function:** Lennard Jones problem
**Cooling schedule:** Lam schedule
**Move Generation:** Lam schedule
**Stopping Criterion:** If Energy change in every M steps smaller than frozen_karpa for consecutive 3 times, the PSA process will be terminated.

## Parallel Simulated Annealing

**Mixing Pattern:** 1-to-all, CDR
**Mixing Period** (MX step) **:** a fixed number range from 1 to 20

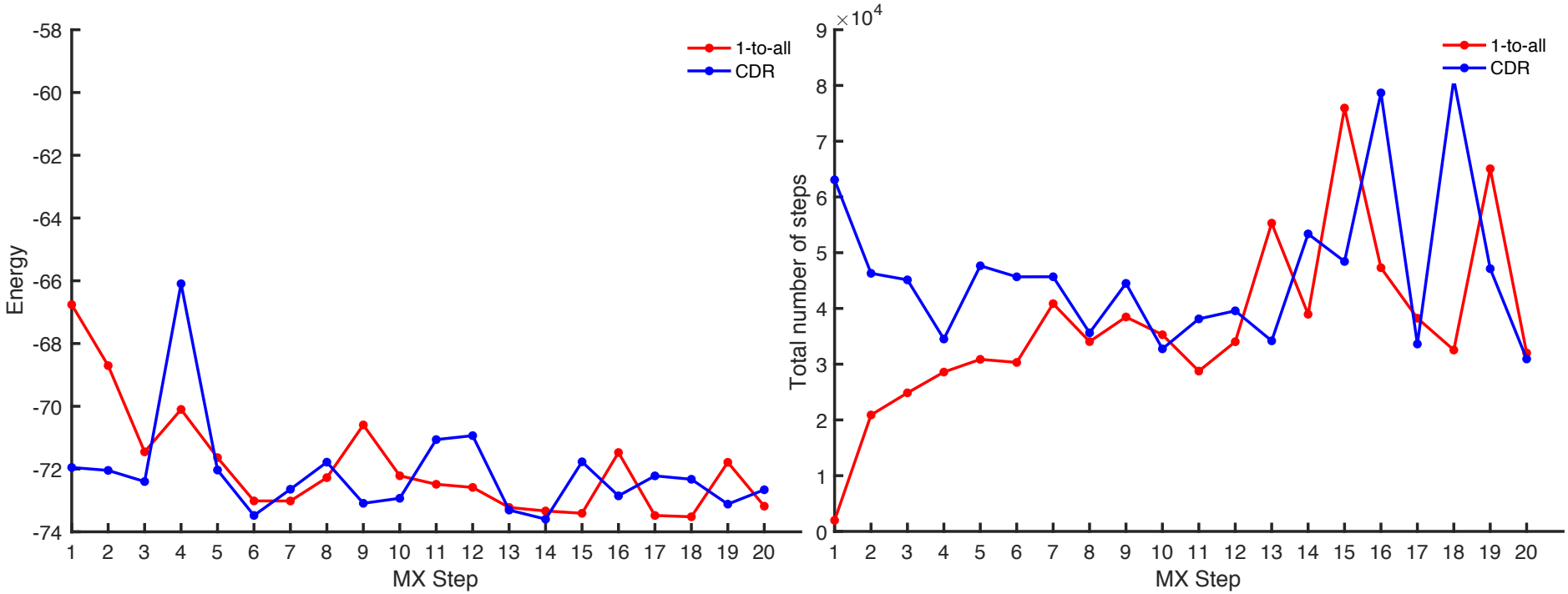
## Aim

To observe the phenomena of the greediness in different mixing pattern and mixing period

**Greediness:** A PSA process achieves a higher energy in a smaller total number of steps

# PSA Experiments

N=20, core number=5, global minima= -77.177043



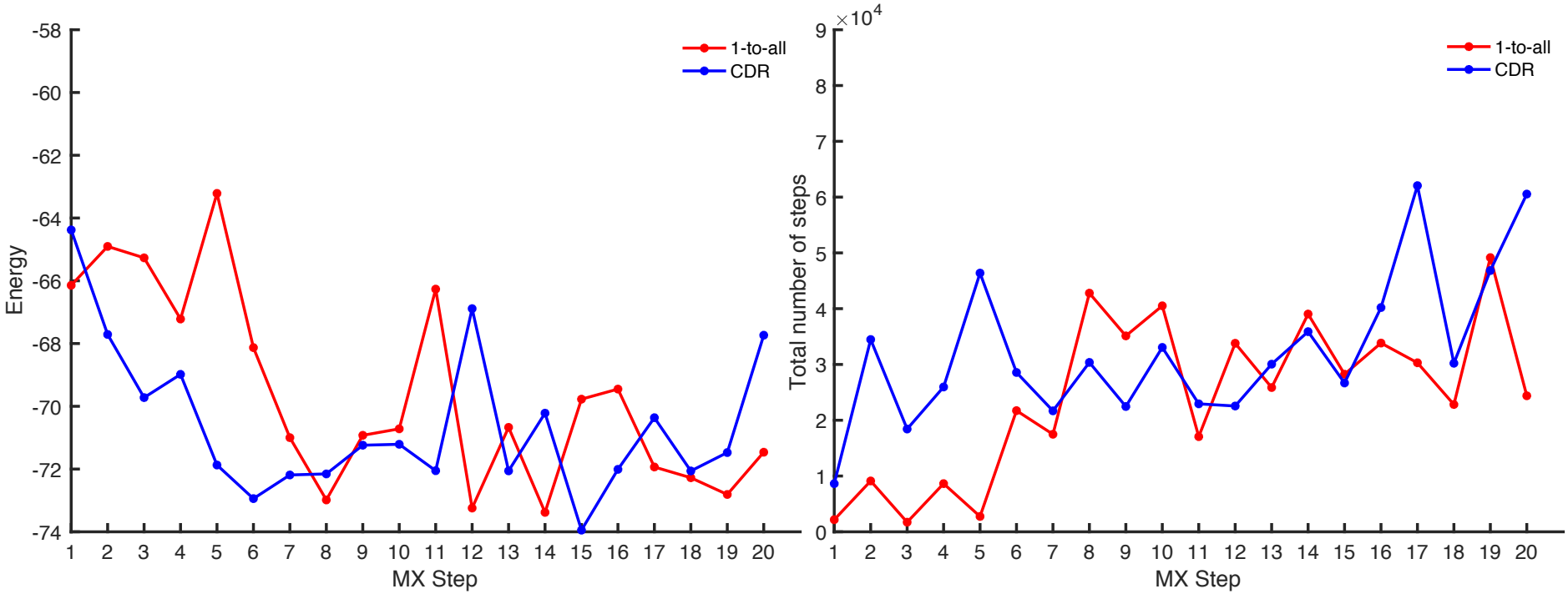

1-to-all: when step is smaller than 2, greedy. the smaller the MX step is, the greedier the PSA process achieve

CDR: MX step does not affect the greediness of the PSA process significantly

1-to-all & CDR: 1-to-all is greedier than CDR

# PSA Experiments

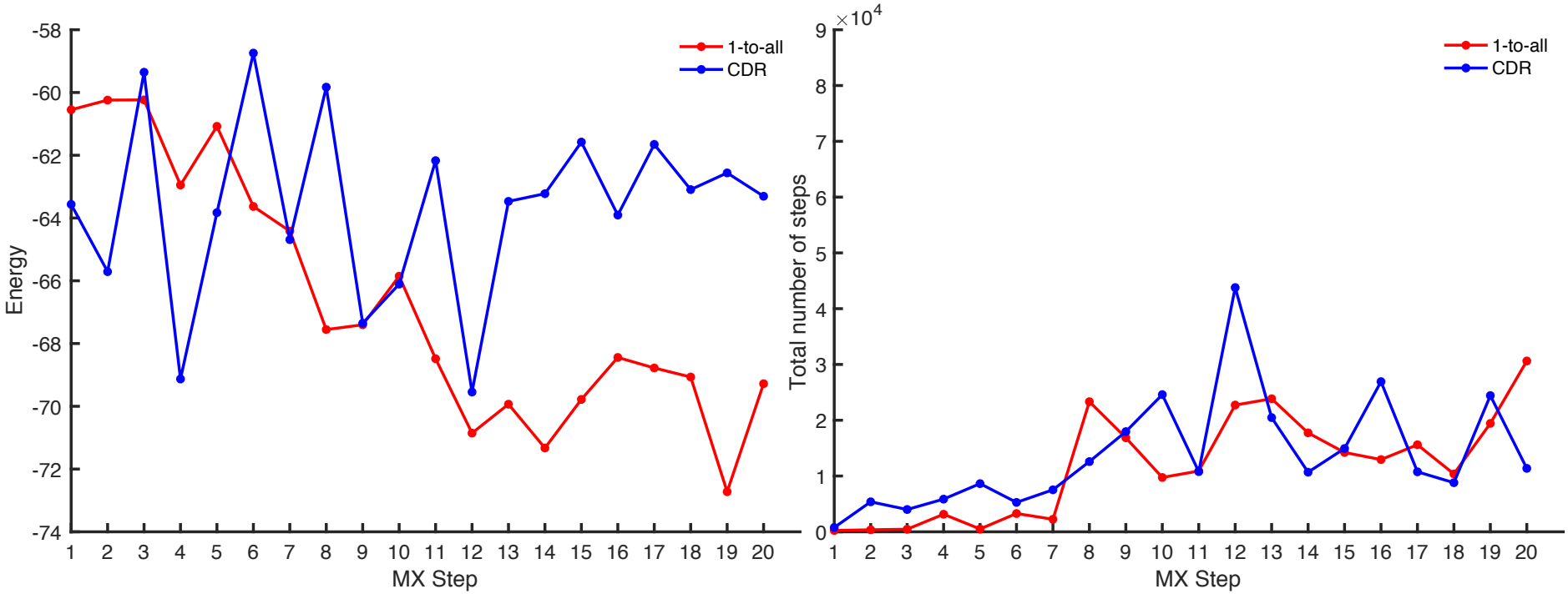
N=20, core number=10, global minima= -77.177043




1-to-all: the first five points as we expected is greedier(higher energy smaller steps than before). As for the rest 15 steps, we only see fluctuation, we think that it won't affect the result a lot.
CDR: MX step does not affect the greediness of the PSA process significantly
1-to-all & CDR: 1-to-all is greedier than CDR

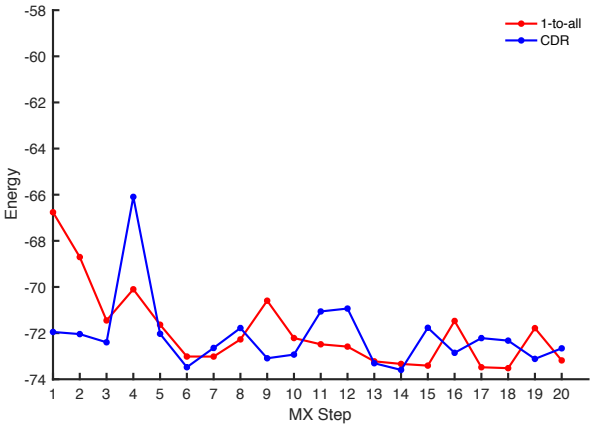
# PSA Experiments

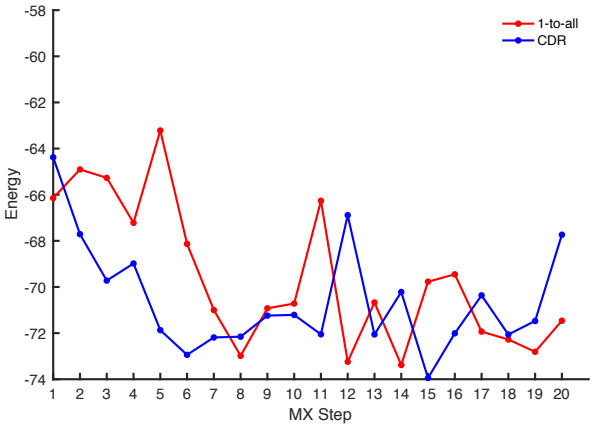
N=20, core number=20, global minima= -77.177043

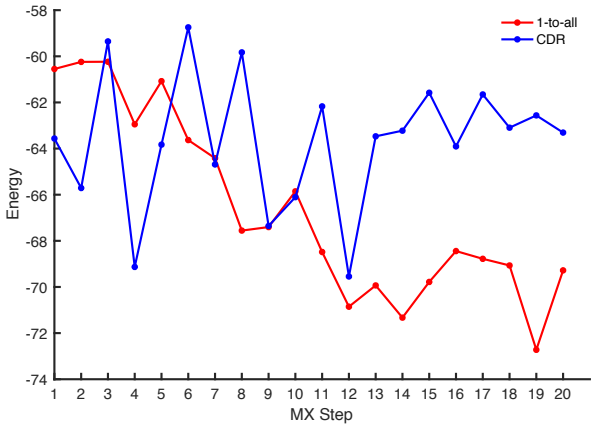


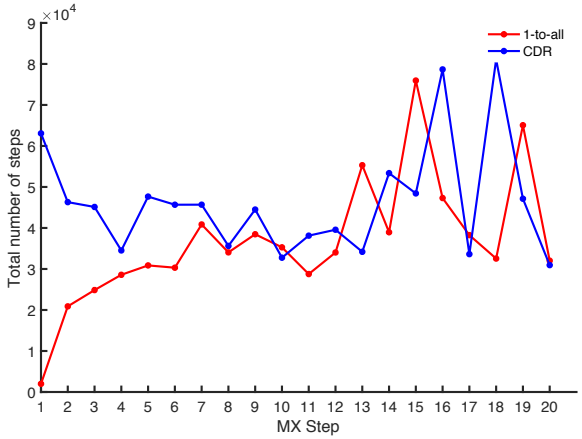

1-to-all:at the beginning, it is very greedy; fluctuate a little at the rest of steps
CDR: tends to be flat
1-to-all & CDR: 1-to-all is greedier than CDR

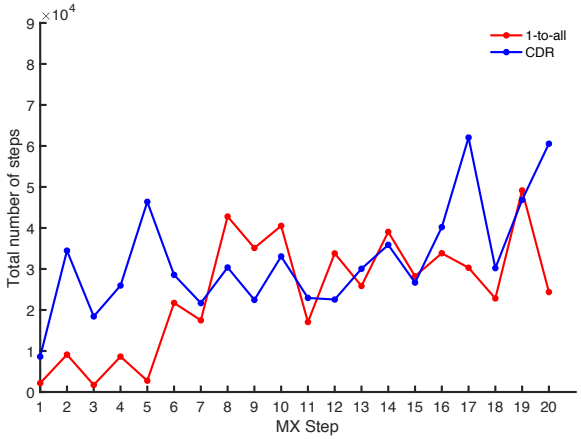
# Observations

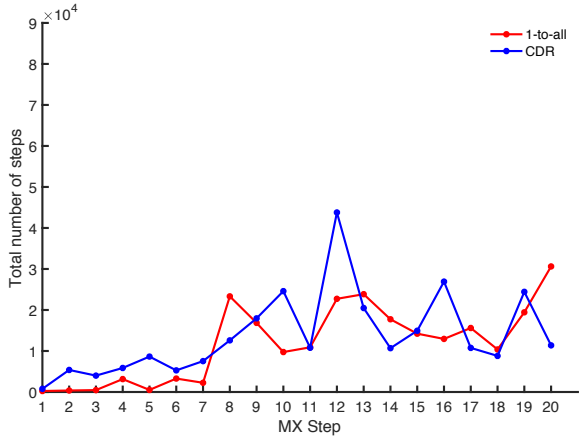


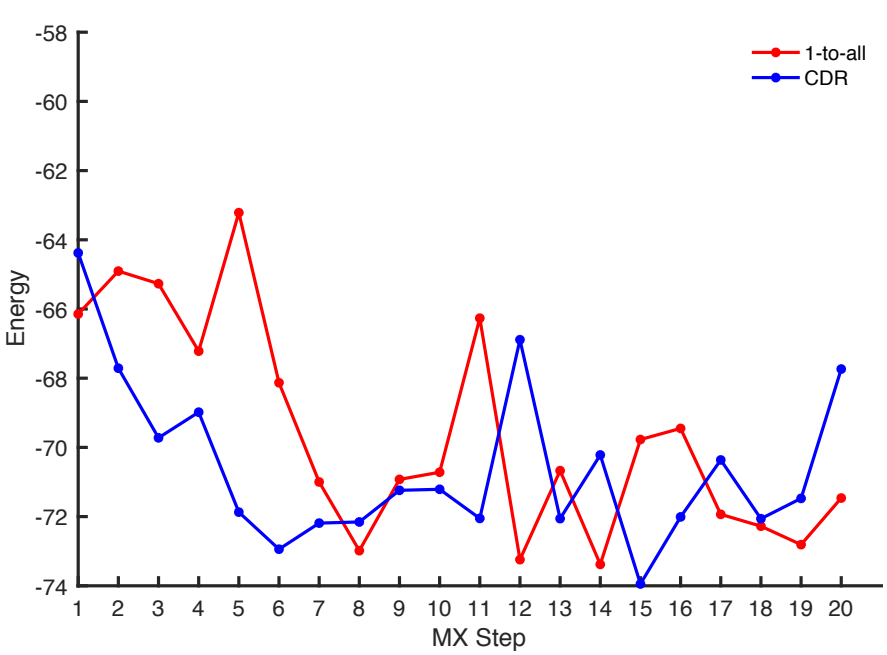



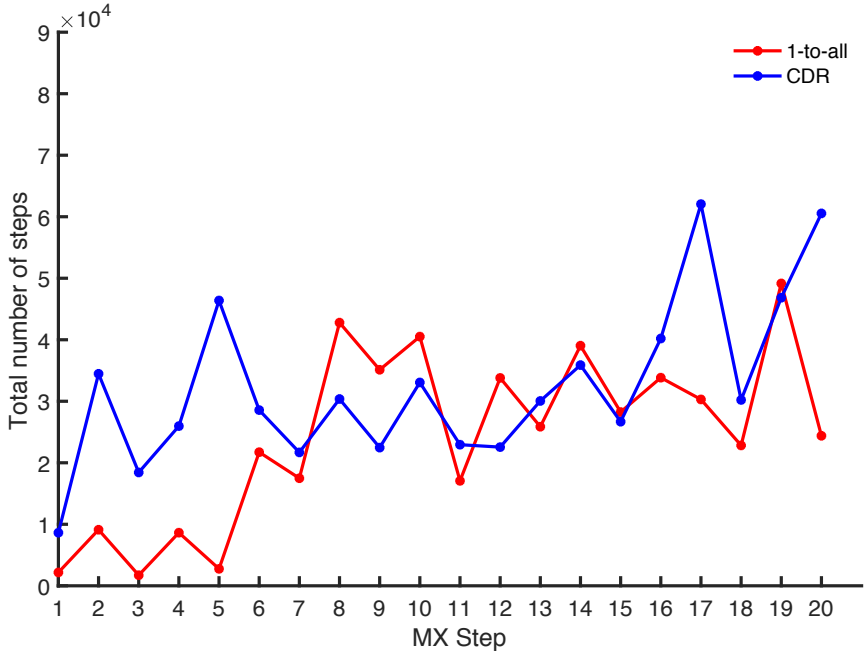

N=20, core number=5 N=20, core number =10 N=20, core number =20

The more the core number has, the greedier the final results a PSA process will achieve

# PSA Experiments

N=20, core number=10, global minima= -77.177043



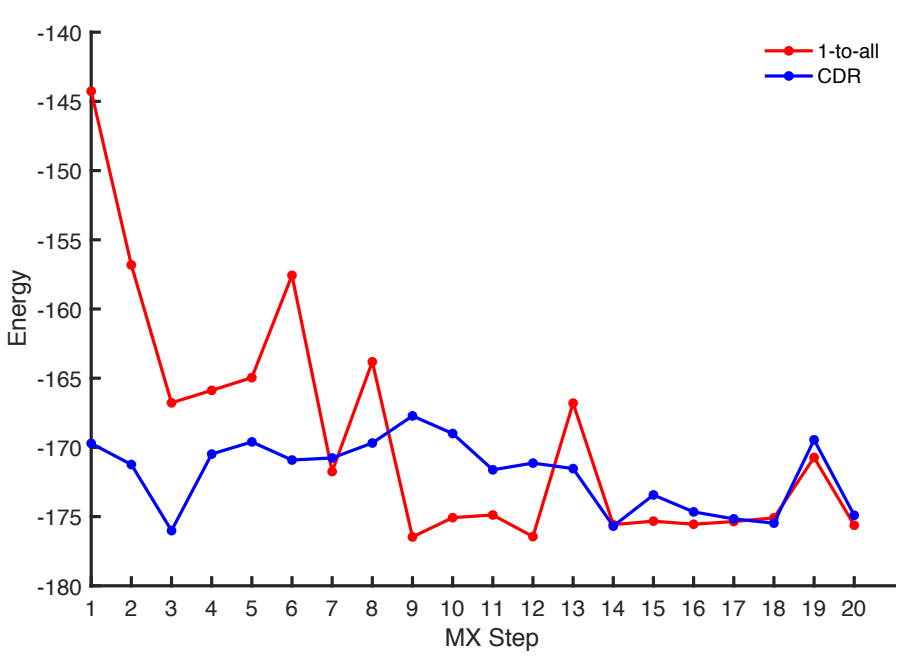

1-to-all: at the first four point, it is greedy because it has high energy and small steps

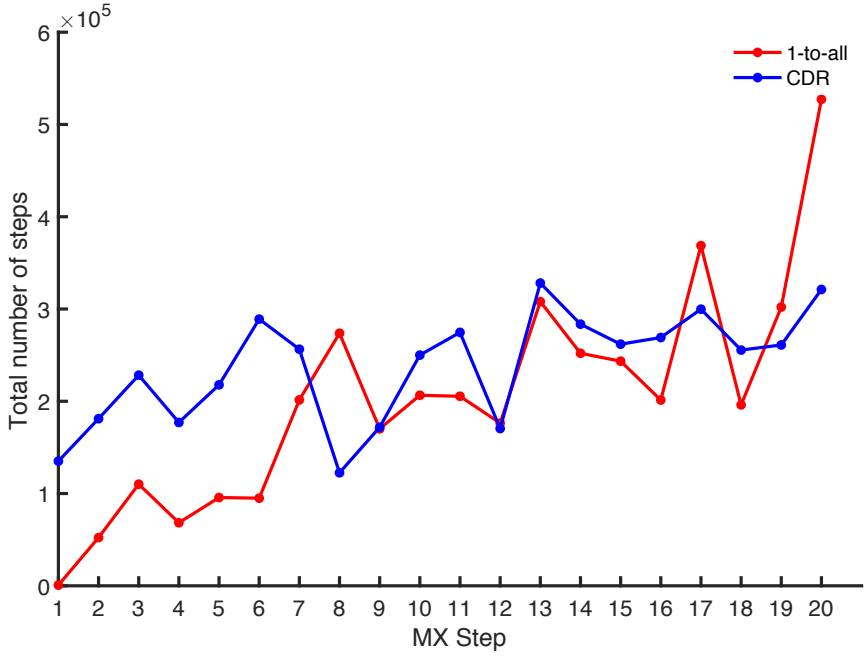
CDR: the first point has clearly high energy and small steps, the other steps tend to flat

1-to-all & CDR: MX Step affect more on 1-to-all than CDR

# PSA Experiments

N=40, core number=10, global minima= -185.249839

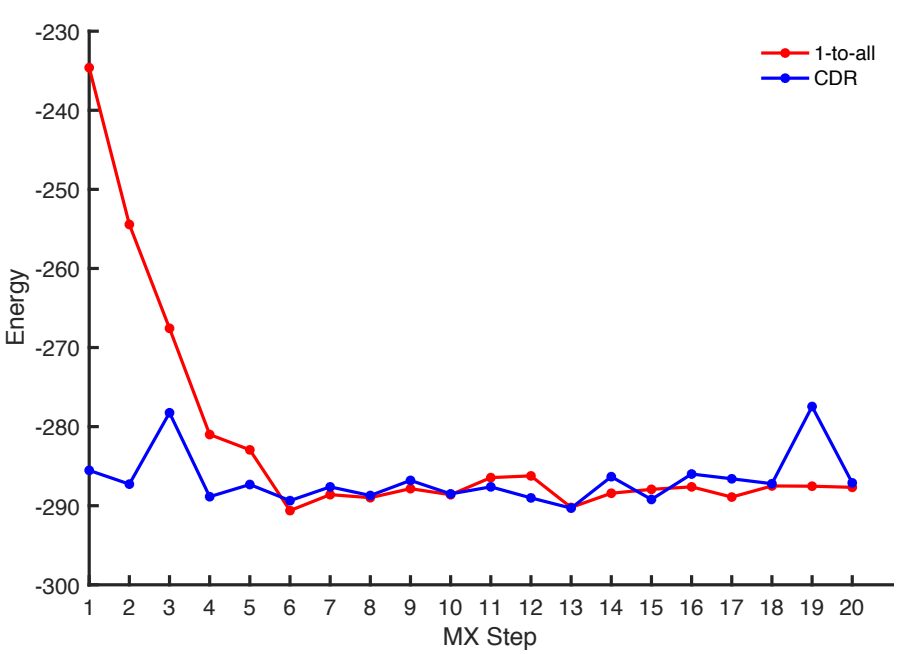


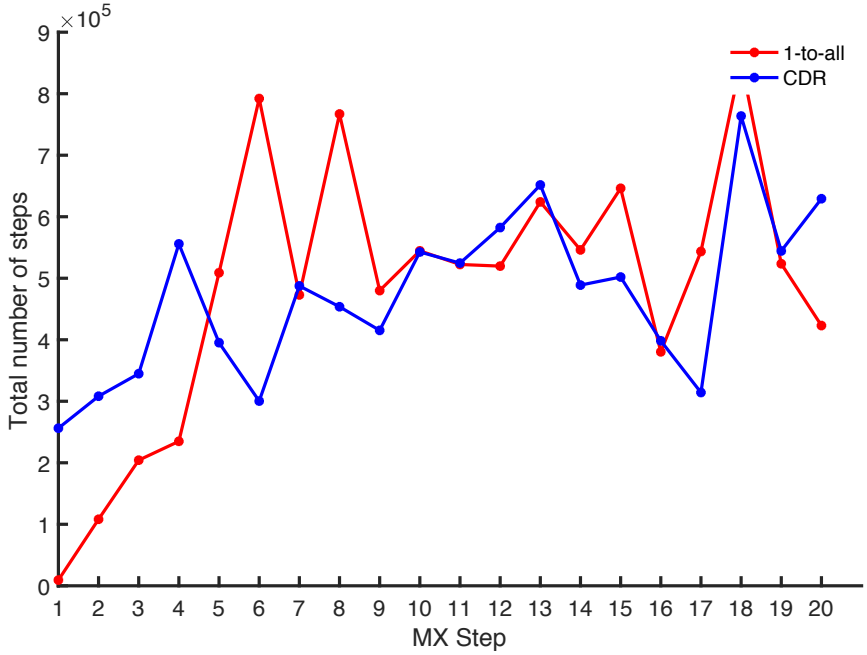




1-to-all: when MX Step is smaller than 6, high energy with small steps
CDR: fluctuation is flat
1-to-all & CDR: see 1-to-all fluctuate clearer than CDR, but tend to flat later

# PSA Experiments

N=60, core number=10, global minima= -305.875476

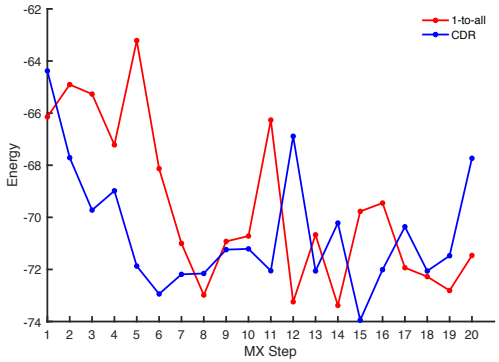


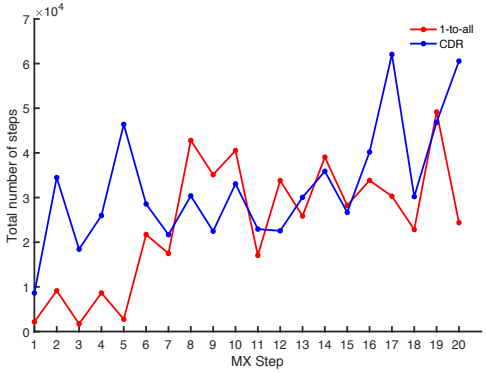




1-to-all: In the first graph, from strongly fluctuate to flat. In the second graph, when step is larger than 4, it fluctuate but still higher than the first 4 point..
CDR: tend to flat
1-to-all & CDR: 1-to-all is sensitive because the first point has higher energy and lower total number of steps. But CDR is not sensitive to mixing steps.

# Observations

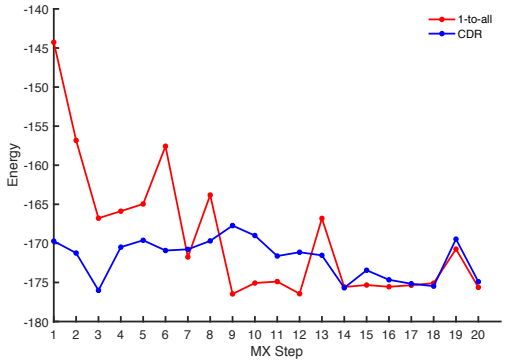
Global minima= -77.177043

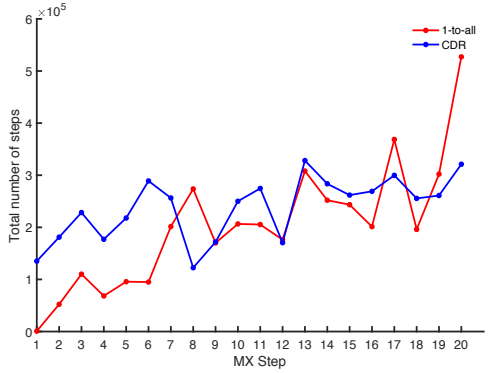



N=20, core number=10

Global minima= -185.249839

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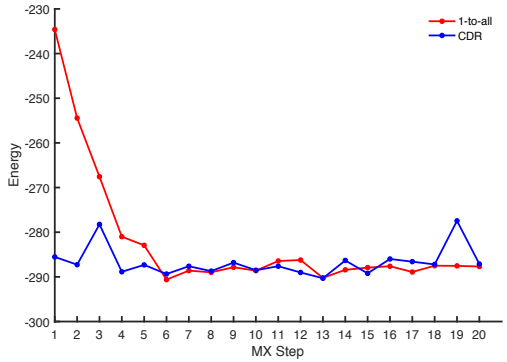


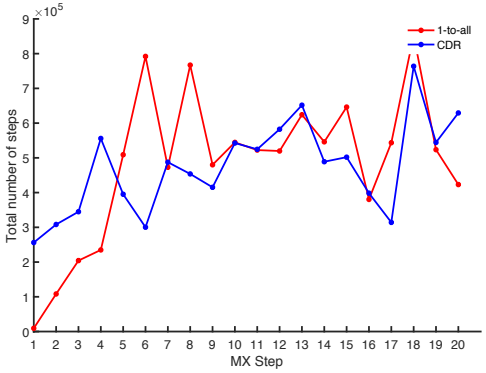


N=60, core number=10

The larger the N is, the greedier the final results a PSA process will achieve

***Thank you!***