Si-Ge Interface Design Using Monte Carlo Tree Search

Thaer M. Dieb[1], Kazuki Yoshizoe[2], Shenghong Ju[3], Junichiro Shiomi[3], Koji Tsuda[2]

[1]National Institute for Materials Science   [2]Graduate School of Frontier Sciences, The University of Tokyo   [3]Department of Mechanical Engineering, The University of Tokyo

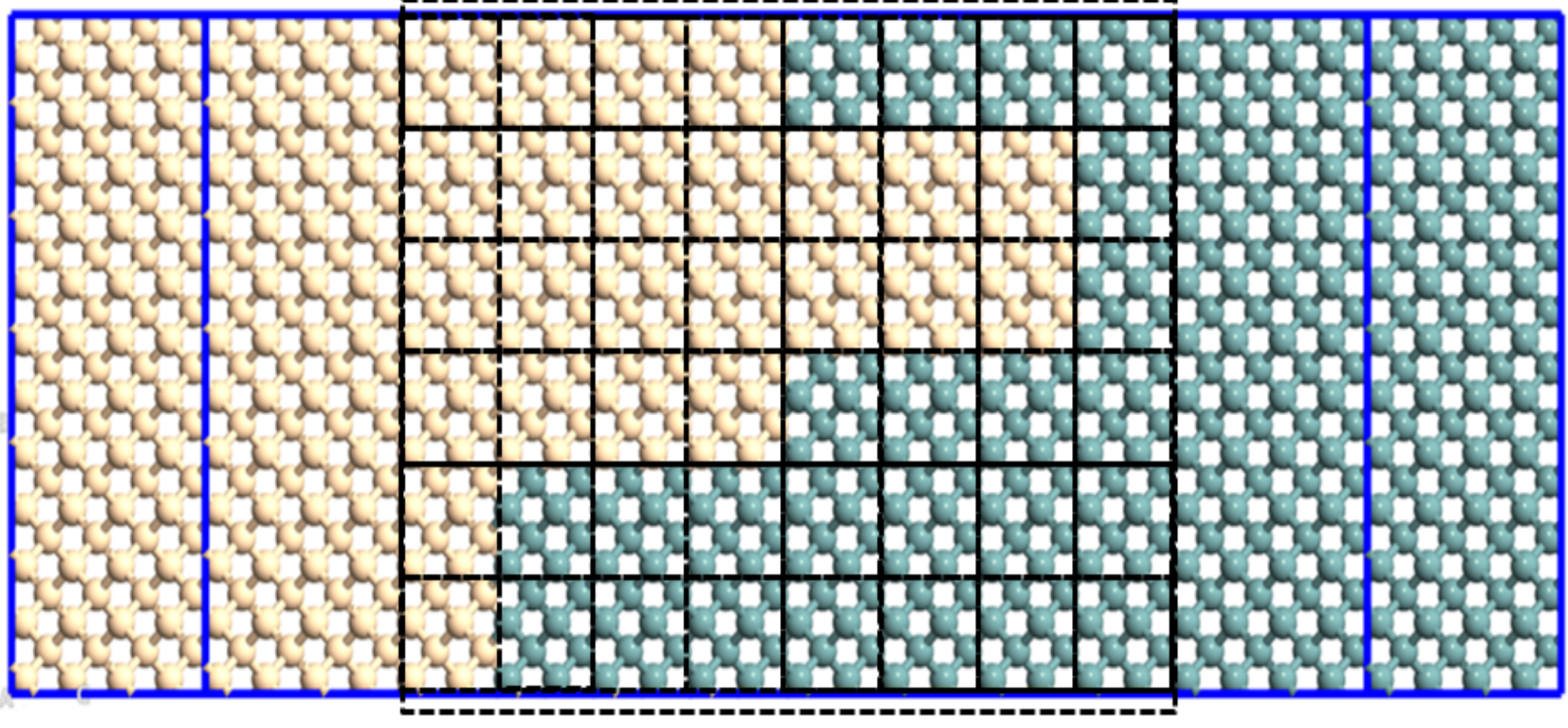[1]MOUSTAFADIEB.Thaer@nims.go.jp
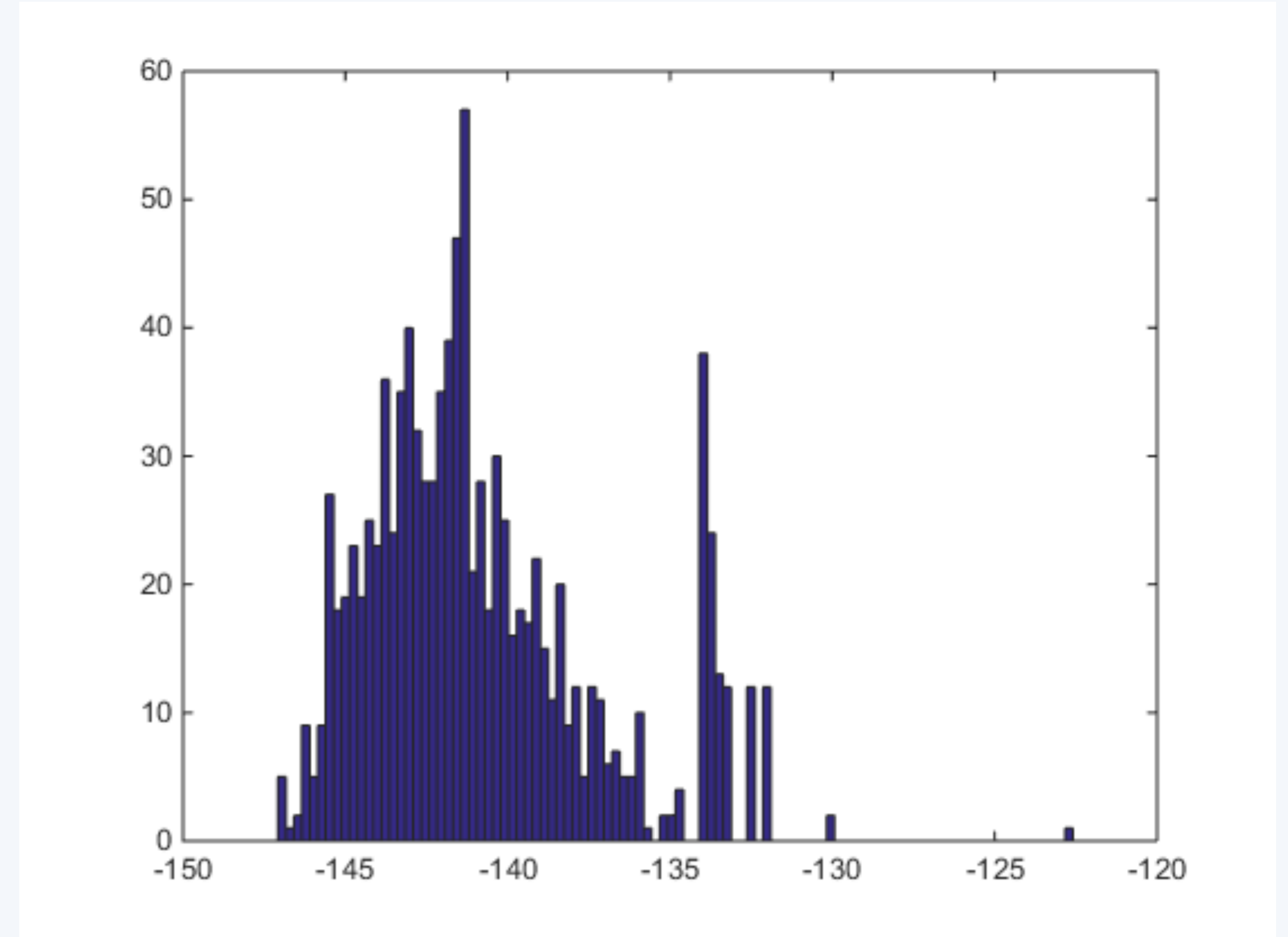
Motivation and Background

Problem definition

Problem example: Arrange 6-layer interface between Si and Ge, keeping Si:Ge ration to 50:50 to obtain the maximum thermal conductance.

🔶 : Si   🔷 : Ge

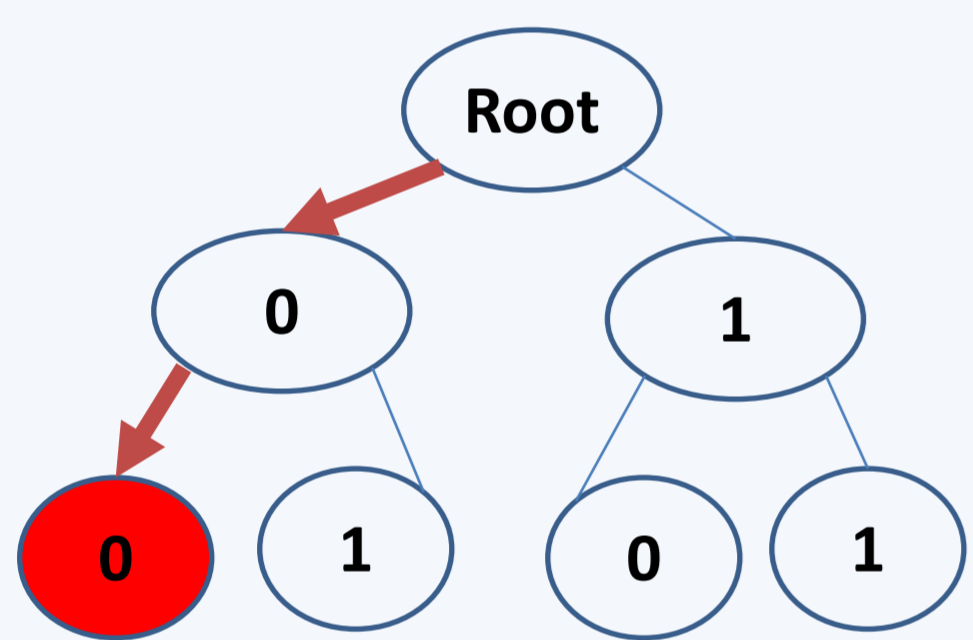**Representation**: The interface in each layer takes a value in [-3,-2,-1,0,1,2,3] with a total sum=0

Number of candidates for 6 layers=6047

Bayesian Optimization (COMBO) is efficient in smaller scale problem, but not so for large scale problems
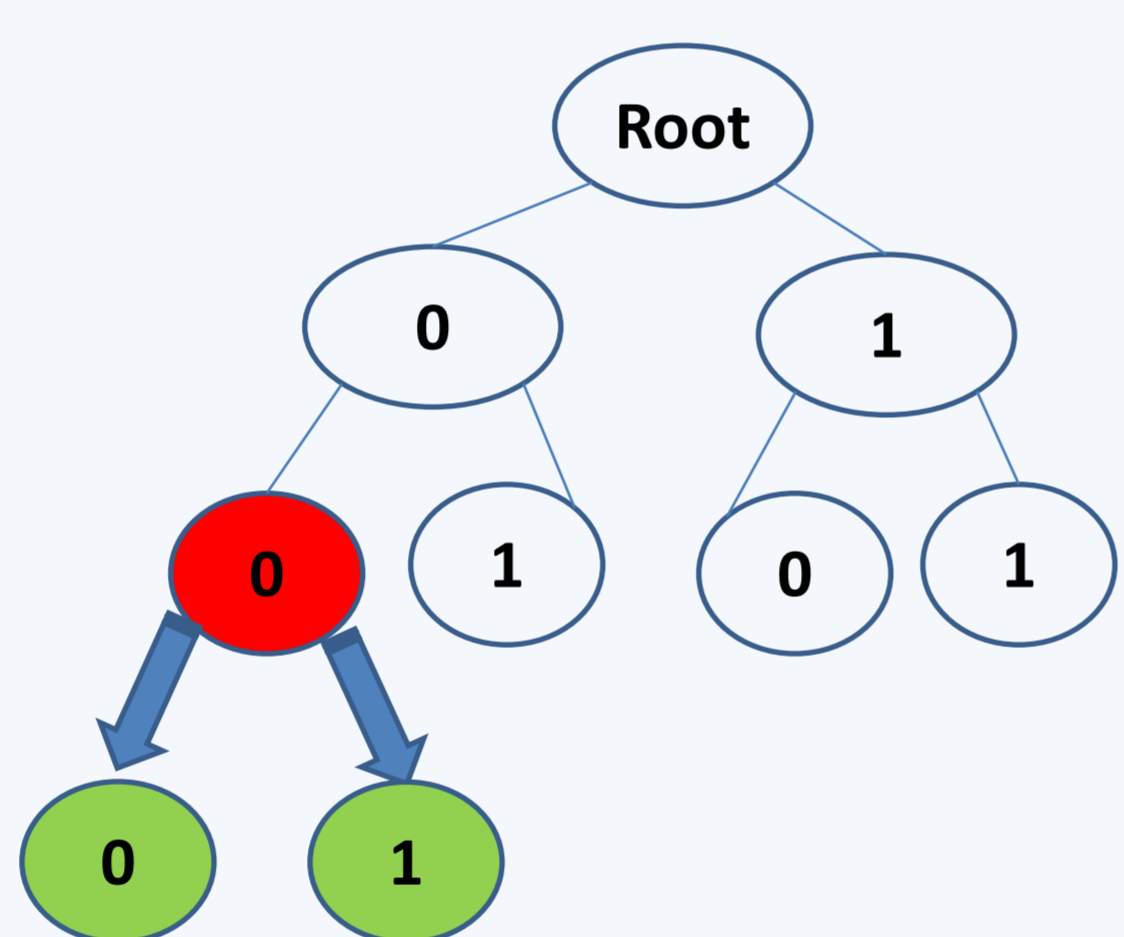
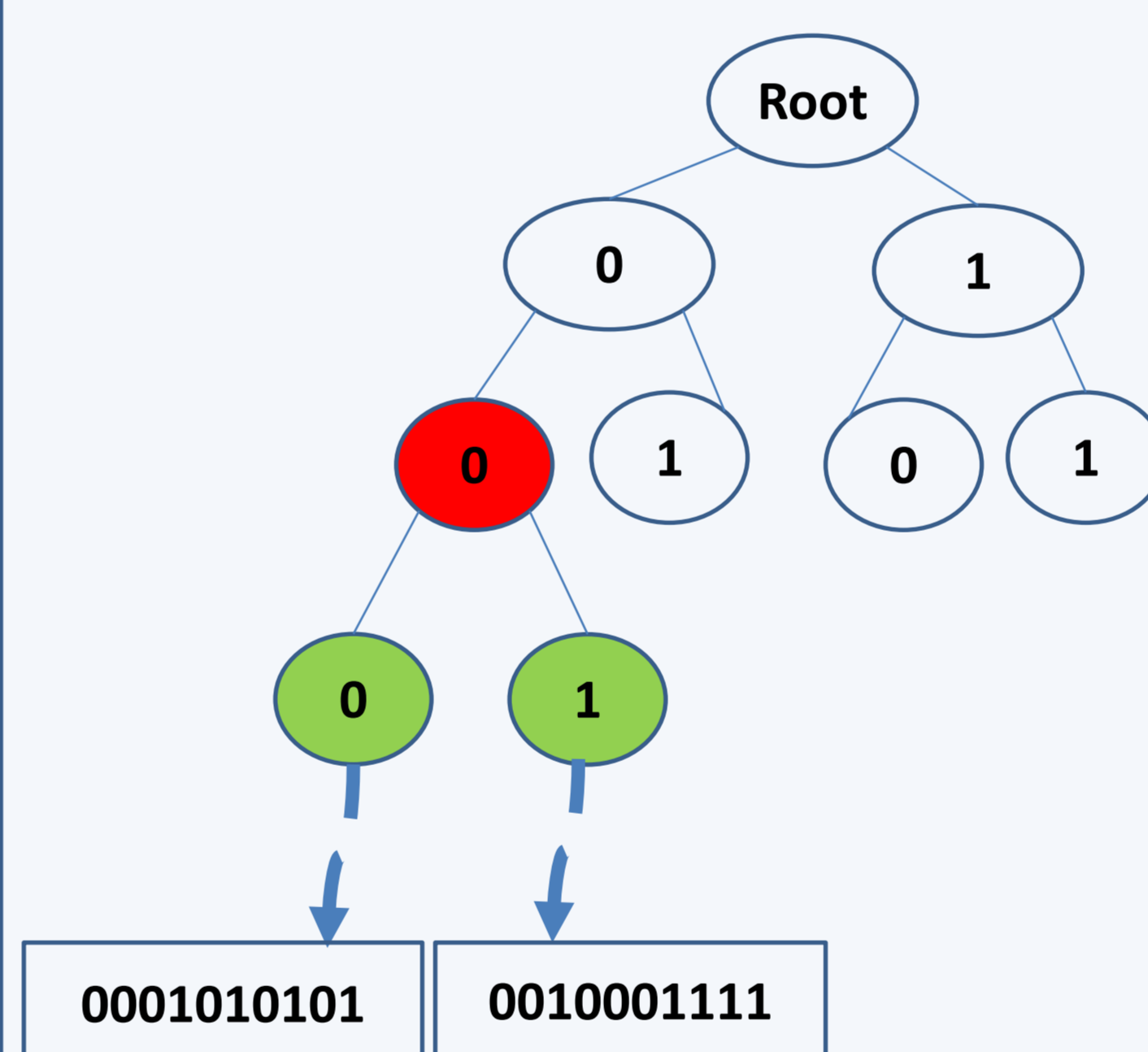## Monte Carlo Tree Search

Selection

Selection criteria

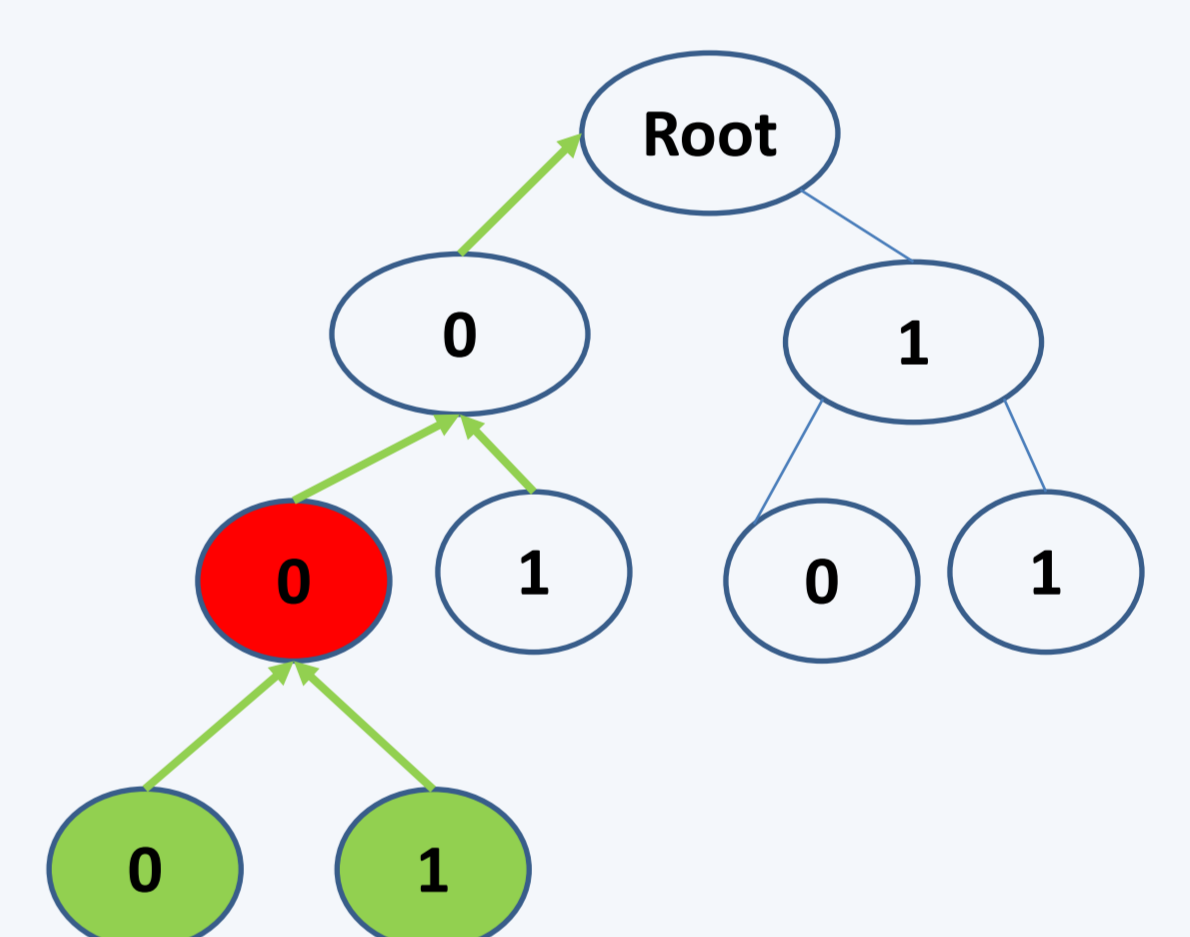$$u_i = \frac{w_i}{v_i} + C\sqrt{\frac{\ln v_{parent}}{v_i}},$$

Expansion

Simulation
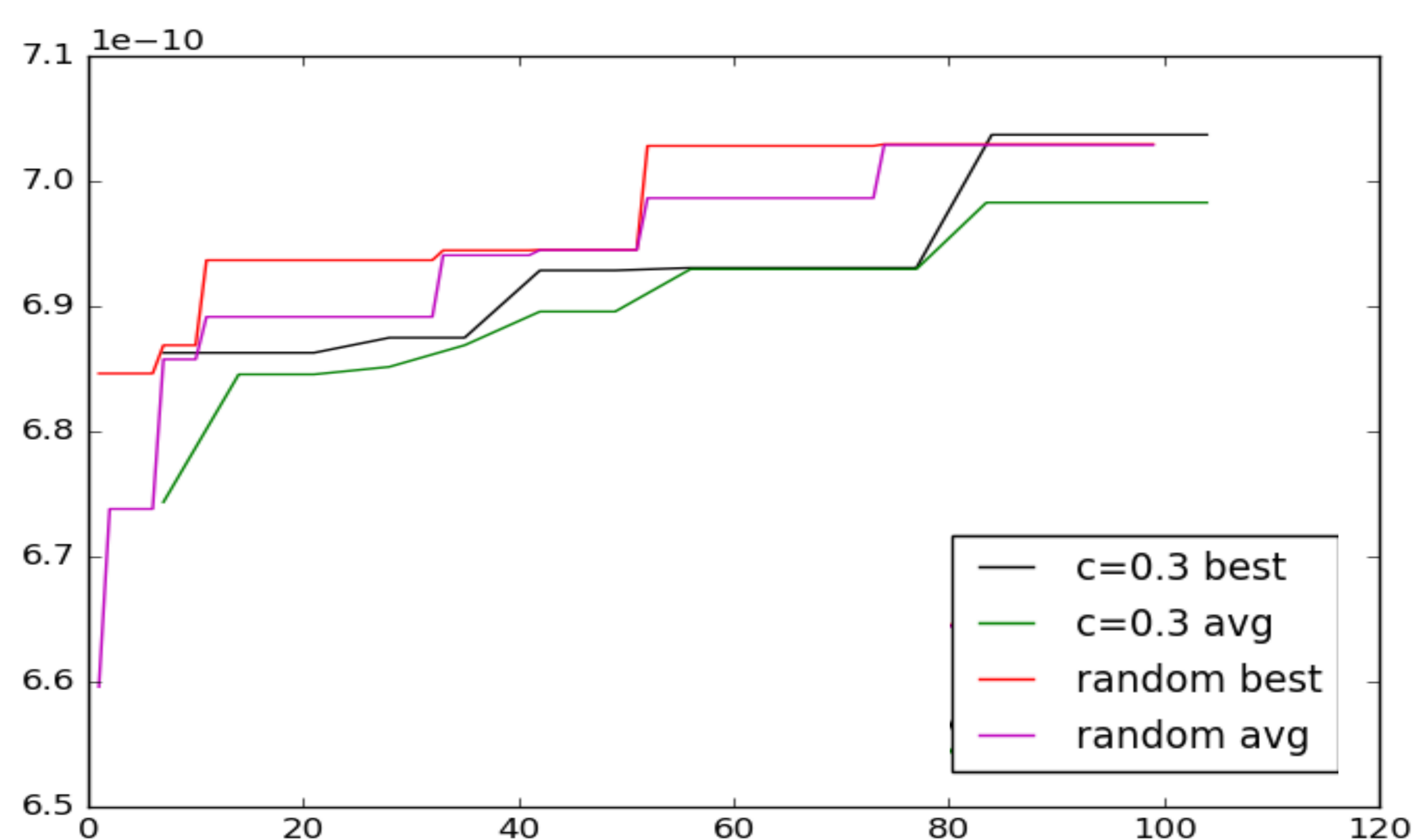

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Backpropagation

Update weight (w) and number of visits (v) using thermal conductance value

Preliminary Experiments' Results

Conclusion & Future Work

We tried Monte Carlo tree search to optimize the design of interface of Si and Ge. Preliminary experiment results does not show significant improvement for MCTS over random search. In the next step, we plan to assess the performance with different hyper parameters for MCTS.