

Supplementary Information for
Predicting the fluid behavior of random microfluidic mixers using convolutional neural networks

Junchao Wang,^{1*} Naiyin Zhang,²
Jinkai Chen,¹ Guodong Su,¹
Hailong Yao,³ Tsung-Yi Ho,⁴ and Lingling Sun¹

¹Key Laboratory of RF Circuits and Systems, Ministry of Education,
and Zhejiang Provincial Laboratory of Integrated Circuit Design,
Hangzhou Dianzi University, China.

²School of Artificial Intelligence, Hangzhou Dianzi University, China.

³Department of Computer Science and Technology,
Tsinghua University, Beijing, China.

⁴Department of Computer Science,
National Tsing Hua University, Hsinchu, Taiwan.

Please find all the following files in github.com/junchaolab/randomCNN.

1 Supplementary files for quantitative analysis of the CNN library

- *qAnalysis.m* is the MATLAB script we used for quantitative analysis of the CNN library.
- *cnnBenchmark.csv* is the raw matching data of 1,000 benchmarks by using the CNN library.
- *randomBenchmark.csv* is the raw matching data of 1,000 benchmarks by using the random library.
- *cnnLibrary.mat* is the MATLAB data file containing the outflow rates and concentrations of 41,270 candidate designs in the CNN library.

- *randomLibrary.mat* is the MATLAB data file containing the outflow rates and concentrations of 10,513 candidate designs in the Random library.

2 Supplementary files for training of neural networks

- *randomAll.csv* is the dataset of all 10,513 pre-simulated random microfluidic mixers, which is used in all the following script.
- *gridInfo.pkl* is the 15x15 matrix/grid information in numpy format of all 10,513 pre-simulated random microfluidic mixers, which is used in all the following CNN training scripts.
- *flowCNN.py* is the Python script we used for training of flowCNN.
- *cCNN.py* is the Python script we used for training of cCNN.
- *ANNVelocity.py* is the Python script we used for training of ANN model to predict three outflow rates. (Described in Section 3.4.1.)
- *ANNConcentration.py* is the Python script we used for training of ANN model to predict three outflow concentrations. (Described in Section 3.4.1.)
- *oneCNNmodel.py* is the Python script we used for training of the single CNN model to predict three outflow rates and concentrations. (Described in Section 3.4.2.)
- *cnnConcentrationThreeOutlets.py* and *cnnConcentrationThreeOutletsNormalized.py* are two Python scripts we used in investigation of necessity of using law of conservation of mass. (Described in Section 3.4.3.)