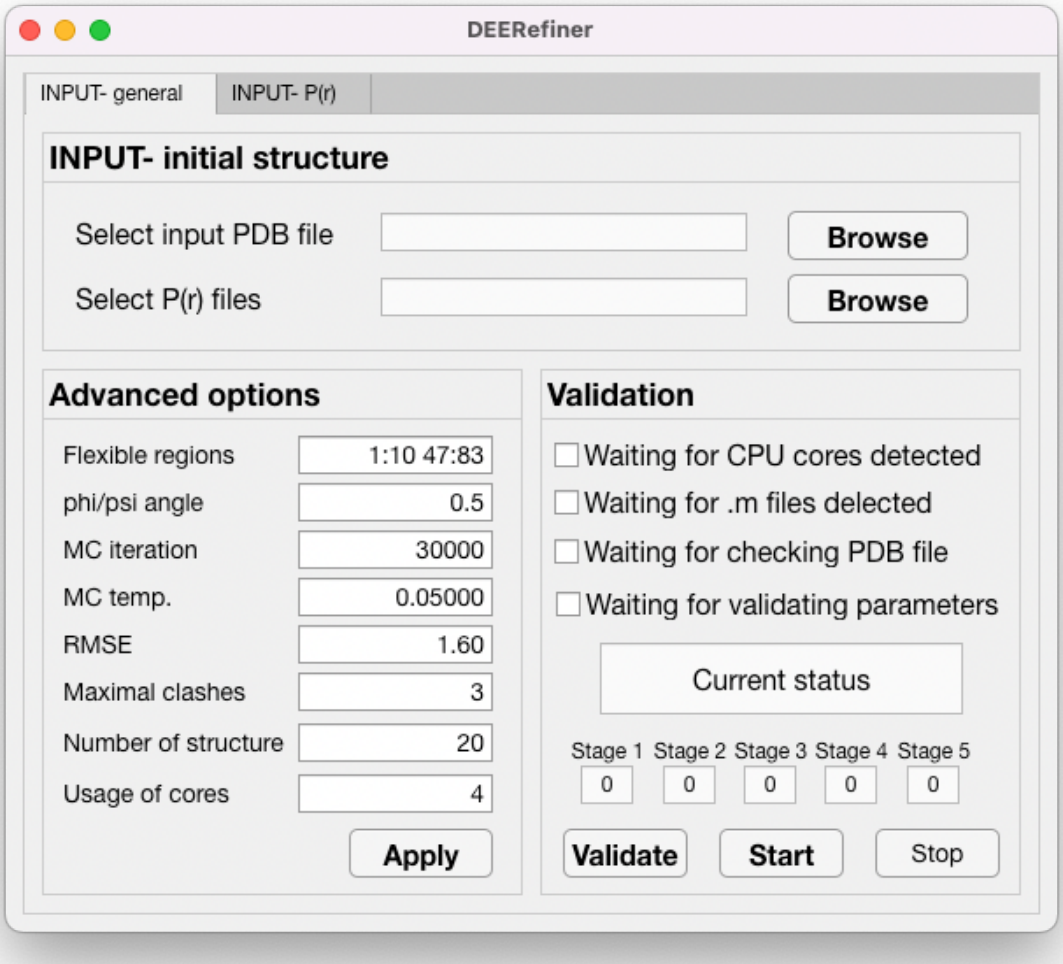
Description

DEERefiner is a MATLAB GUI program for modeling protein ensemble using DEER data.

This program allows biophysists to obtain DEER-derived protein structure.



Built With

MATLAB R2021a on macOS Monterey

Getting Started

Prerequisites

1. MATLAB R2021a or later
2. MATLAB Parallel Computing Toolbox (accelerate drastically)

Installation

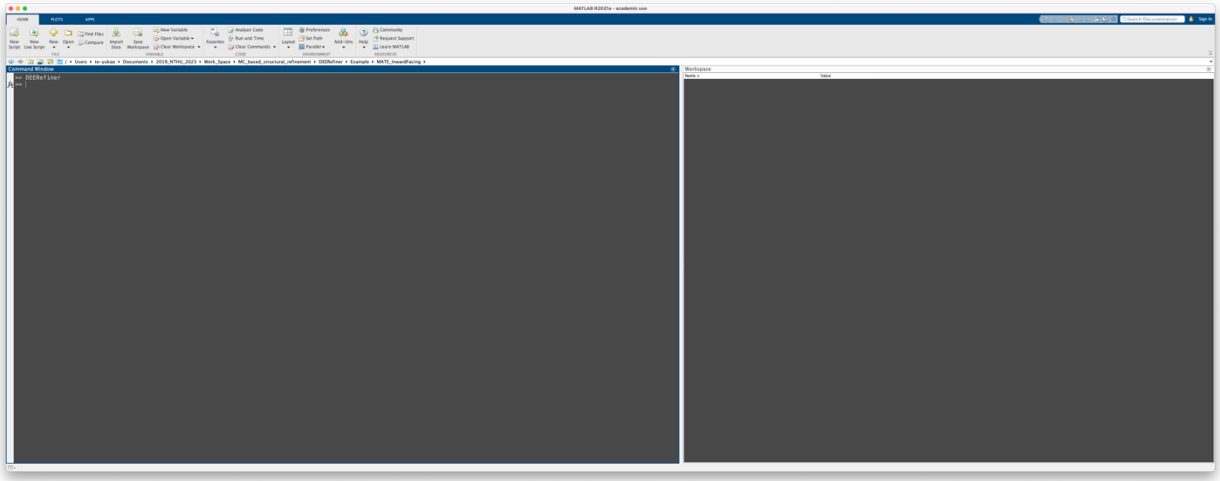
1. Clone the repository (or download the whole folder)

```
# Download the DEERefiner folder
git clone https://github.com/havebeen/DEERefiner/
```

2. Set the DEERefiner folder to your MATLAB path

Usage

```
% Launch DEERefiner GUI in MATLAB
DEERefiner
```



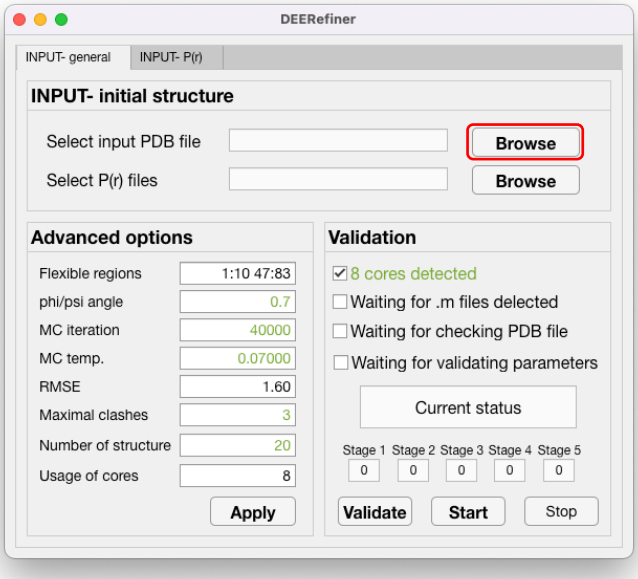
Step 1- Loading PDB file

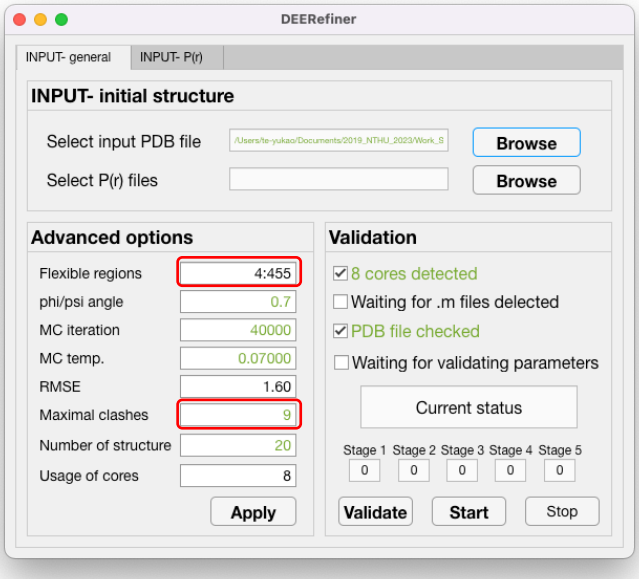
DEERefiner supports almost all PDB files from different resources, including NMR, Cryo-EM, crystallography, and AlphaFold.

Note that, DEERefiner utilizes the first conformation while using NMR structre as the input.

DEERefiner mutates residues with unresolved side chain to alanine.

1. Load the PDB file by clicking **"Browse"** at Select input PDB file.
2. After you load the PDB file, some parameters are determined automatically by DEERefiner, including Flexible regions and Maximal clashes.

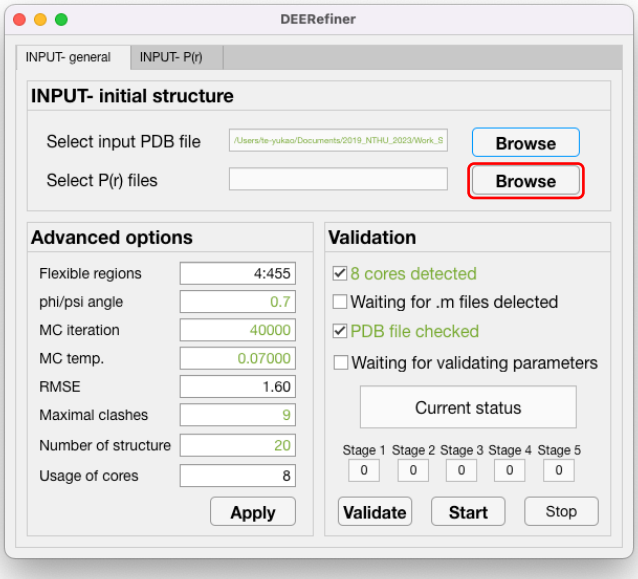




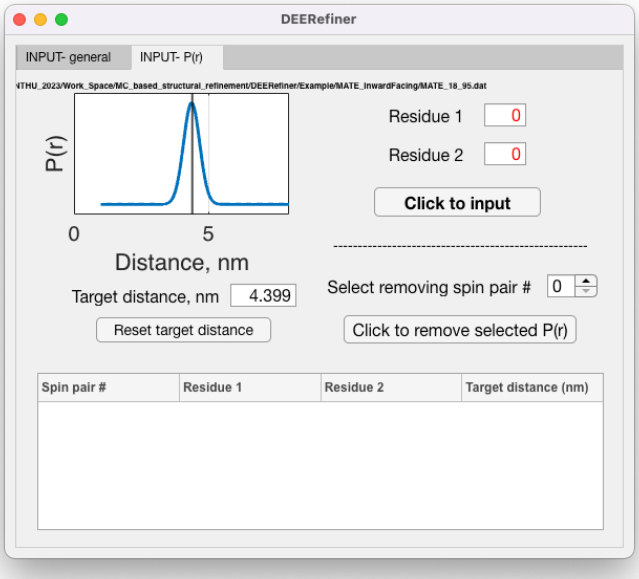
Step 2- Loading distance distribution files (supporting all ASCII file with distance in nm as first column and probability as second column)

DEERefiner supports all ASCII file with distance in nm as first column and probability as second column, such as files from DeerAnalysis or
see `Example/MATE_InwardFacing/MATE_18_95.dat`.

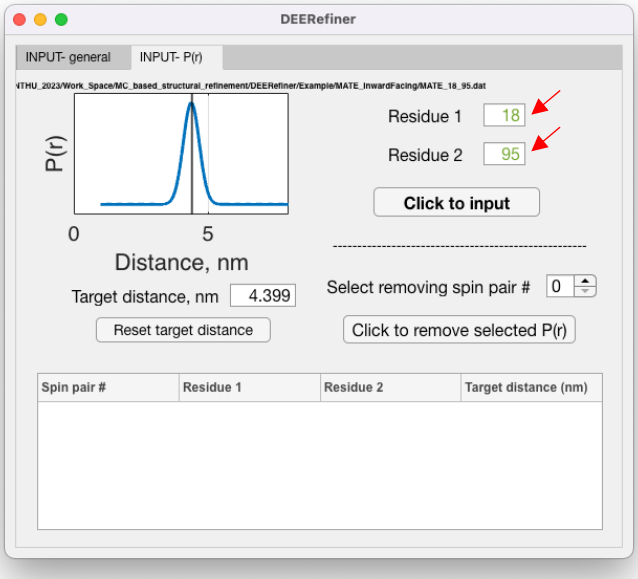
1. Load the distance distribution file by clicking **"Browse"** at Select P(r) file.



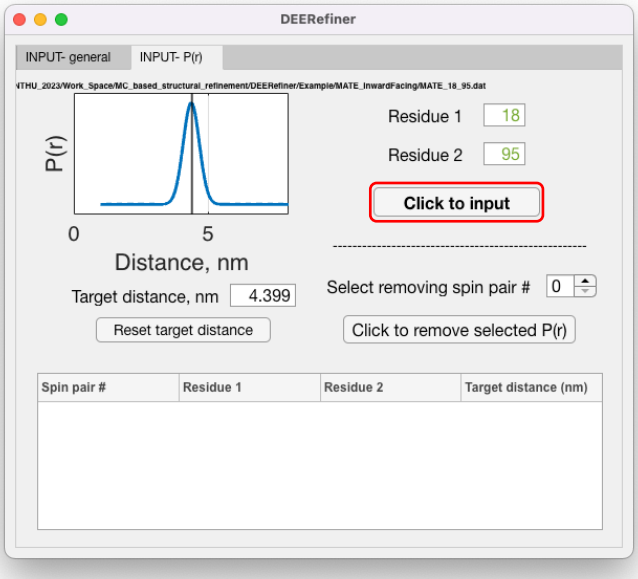
2. Selecting target peaks by left clicking your mouse.



3. Input corresponding residues of this distance distribution.



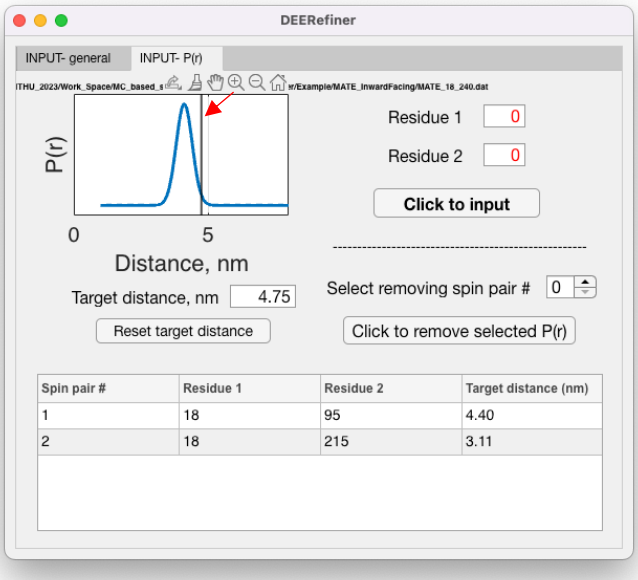
4. Input the data by clicking **"Click to input"**.



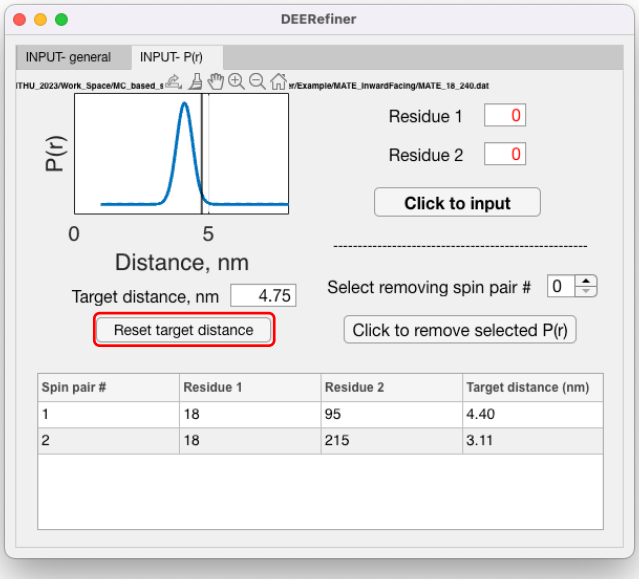
Step 3- Reselect target distance (optional)

Users can reset the target distance.

1. Wrongly determined target distance, clearly the target is not located at the maximum.



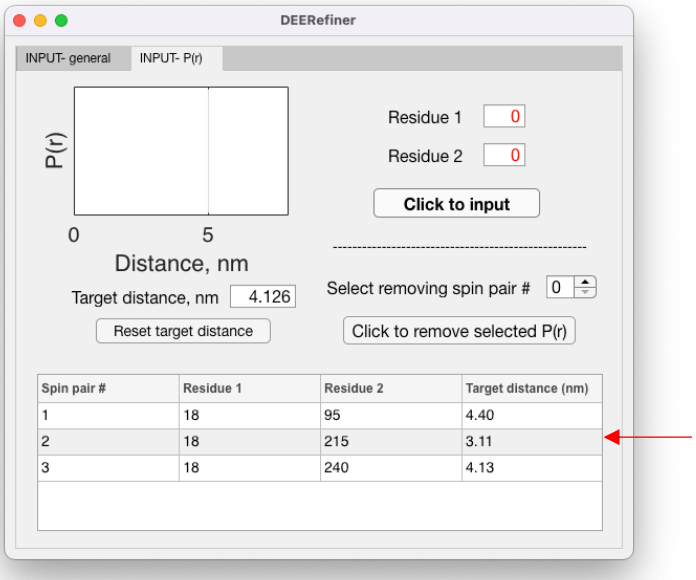
2. Reset the target by clicking **"Reset target distance"**.



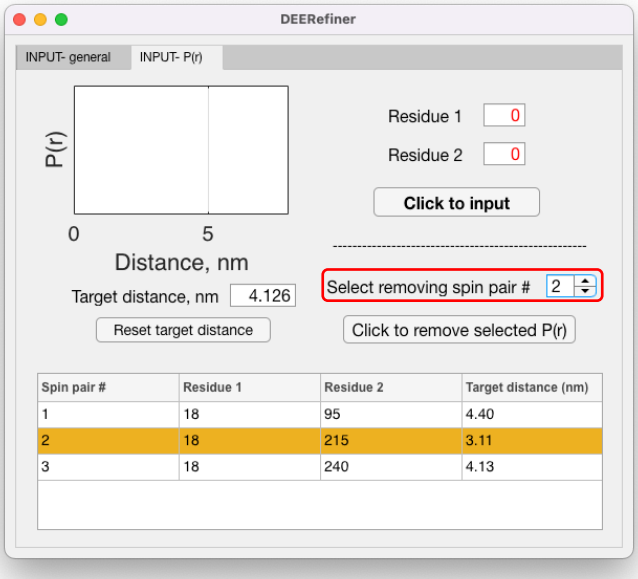
Step 4- Removing wrongly-loaded distance distribution files (optional)

Users can use the feature to remove wrongly-loaded distance distribution.

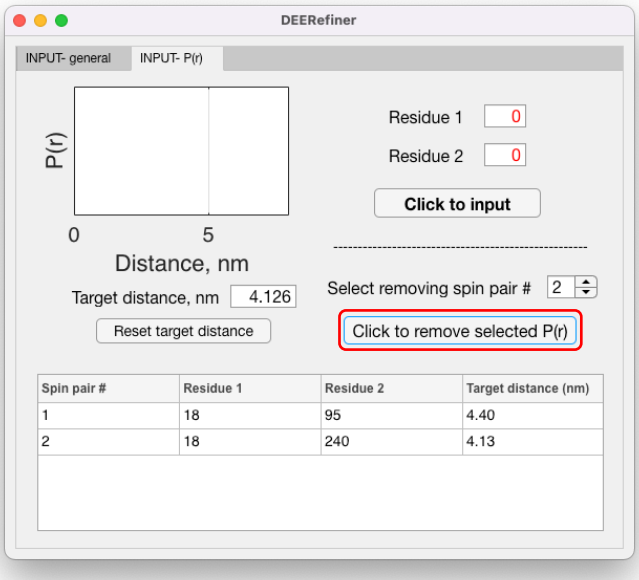
1. Wrongly loaded spin pair.



2. Select the spin pair you want to remove by the spinner.



3. Remove wrongly loaded P(r) by clicking **“Click to remove selected P(r)”**.



Step 5- Setting parameters

All parameter will be determined after loading PDB file and all distance distribution files.

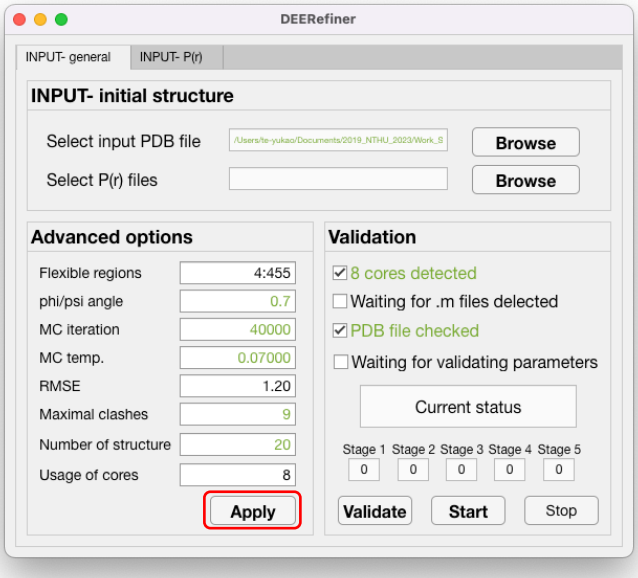
However, the definition of each parameter are listed below in case users want to change them manually.

1. Flexible regions: Residue index with rotatable peptide bonds during simulation.
2. phi/psi angle: Peptide bonds rotating angle at each step.
3. MC iteration: Number of Monte Carlo steps.
4. MC temp.: denominator of the Boltzman factor exponent of Monte Carlo algorithm, larger the MC temp., more easily to escape local minimum.
5. RMSE: Root mean square error criterion for determining convergence, smaller the RMSE, harder to converge.
6. Maximal clashes: Clashed side chain criterion. Clashed residues should be minimized if further simulations will be performed.
7. Number of structure: Total structure will be generated by DEERefiner.
8. Usage of cores: Total CPU cores will be used during simulation.

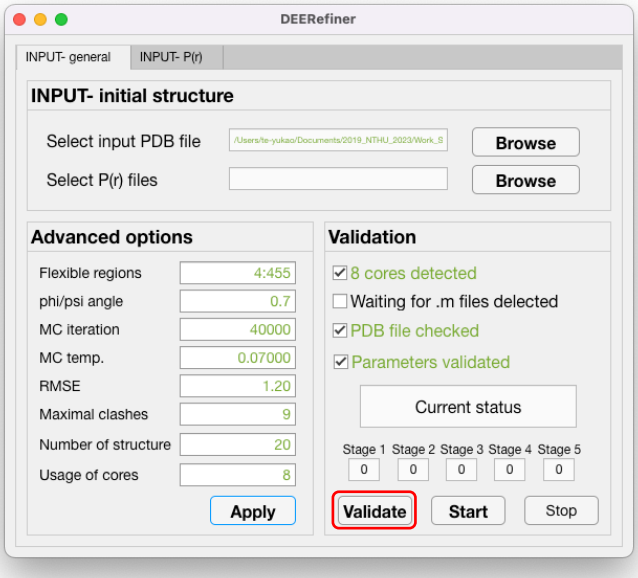
Step 6- Executing simulations

Option 1. Execute simulation with GUI Click the Start buttom.

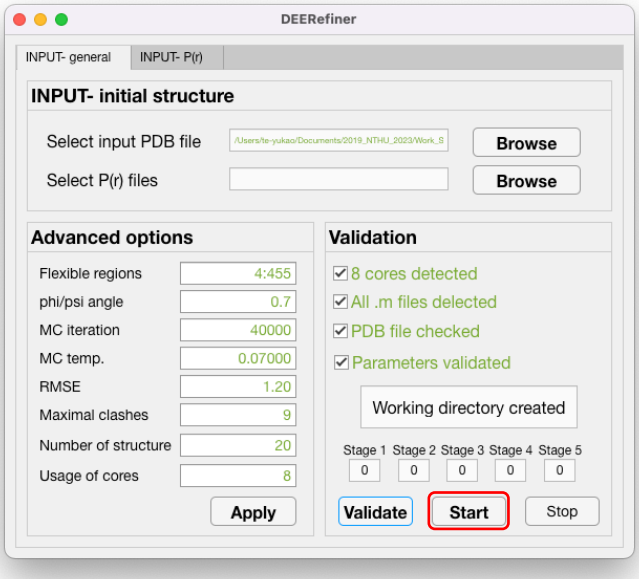
1. Input parameters by clicking **“Apply”**.



2. DEERefiner validates all file by clicking **“Validate”**.



3. Execute simulations by clicking **“Start”**.



Option 2. Execute simulation with command line

```
% simulation execution in MATLAB
Job = runFilesCluterExecutor;
```

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