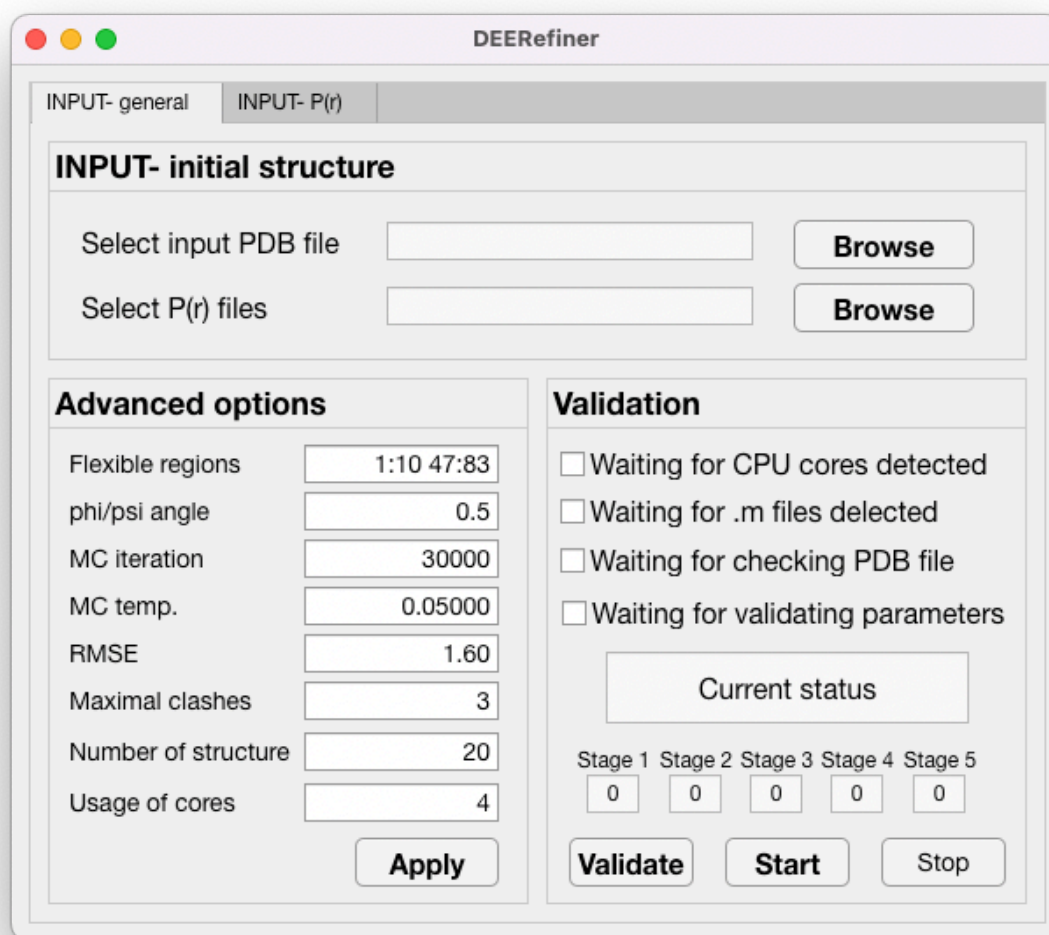


Description

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
3. MATLAB Image Processing Toolbox

Installation

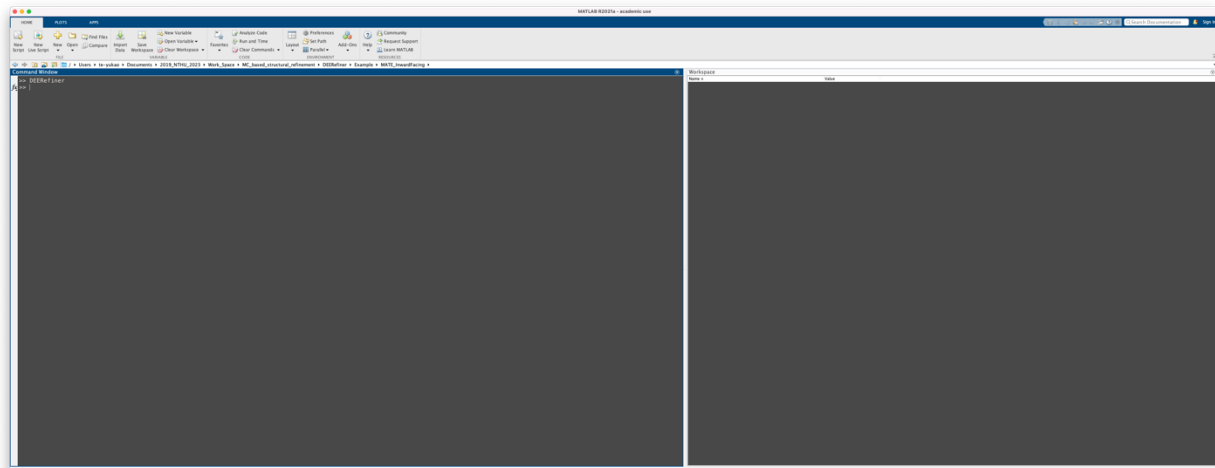
1. Clone the repository (or download the whole folder)

```
# 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
```



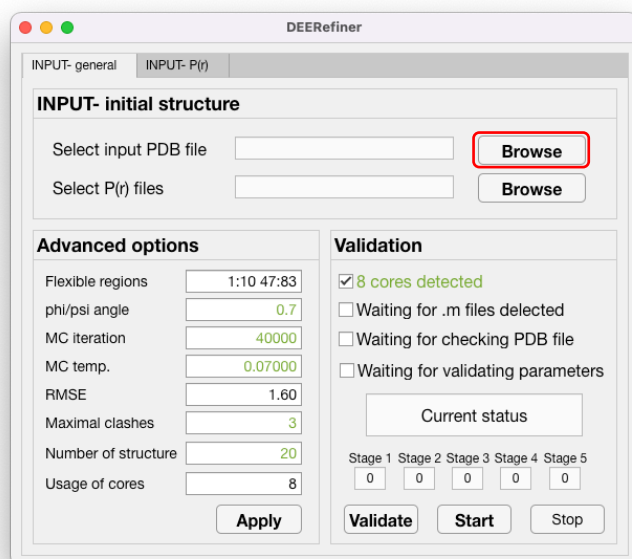
Step 1- Loading PDB file

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 structure 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.



DEERefiner

INPUT- general INPUT- P(r)

INPUT- initial structure

Select input PDB file **Browse**

Select P(r) files **Browse**

Advanced options

Flexible regions

phi/psi angle

MC iteration

MC temp.

RMSE

Maximal clashes

Number of structure

Usage of cores

Validation

☒ 8 cores detected

☐ Waiting for .m files detected

☐ Waiting for checking PDB file

☐ Waiting for validating parameters

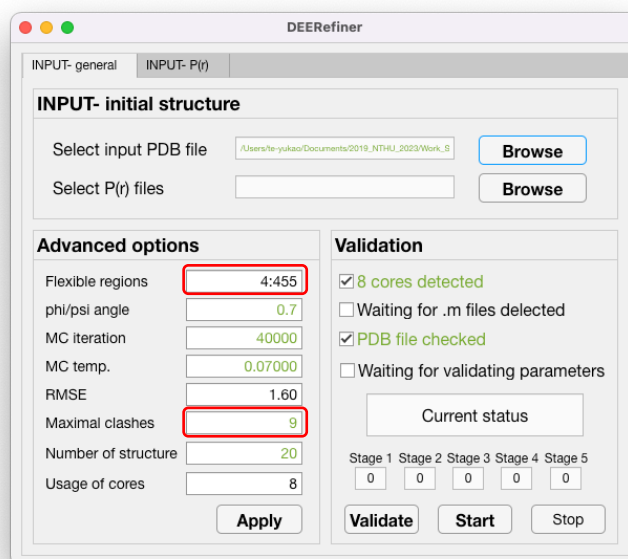
Current status

Stage 1 Stage 2 Stage 3 Stage 4 Stage 5

0 0 0 0 0

Validate Start Stop

Apply



DEERefiner

INPUT- general INPUT- P(r)

INPUT- initial structure

Select input PDB file **Browse**

Select P(r) files **Browse**

Advanced options

Flexible regions

phi/psi angle

MC iteration

MC temp.

RMSE

Maximal clashes

Number of structure

Usage of cores

Validation

☒ 8 cores detected

☐ Waiting for .m files detected

☒ PDB file checked

☐ Waiting for validating parameters

Current status

Stage 1 Stage 2 Stage 3 Stage 4 Stage 5

0 0 0 0 0

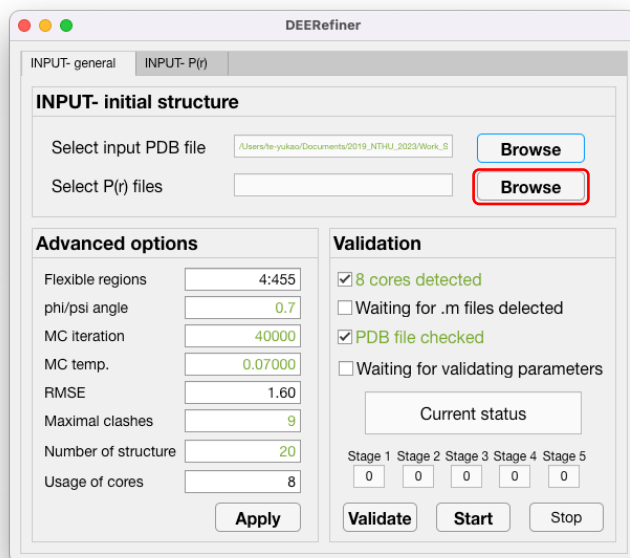
Validate Start Stop

Apply

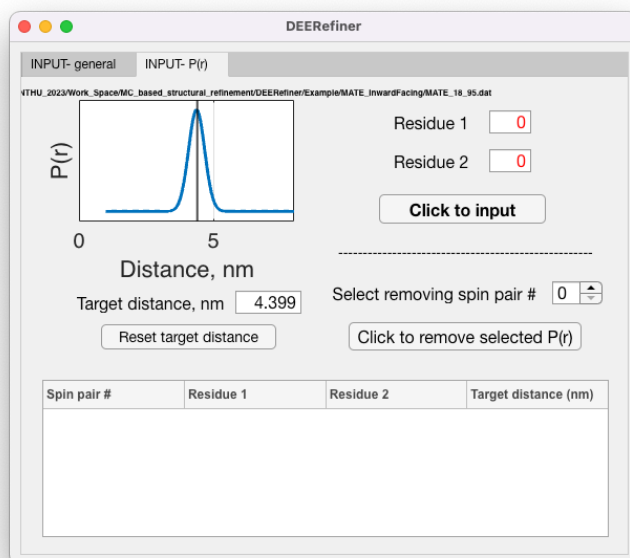
Step 2- Loading distance distribution files (supporting all ASCII file with distance in nm as first column and probability as second column)

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.

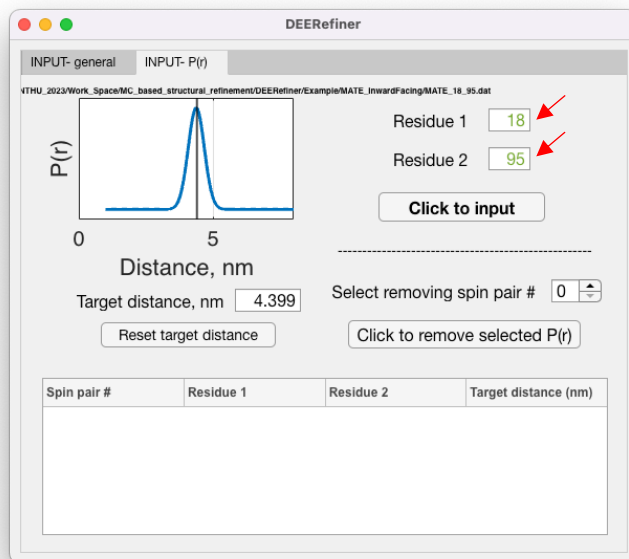
1. Load the distance distribution file by clicking “**Browse**” at Select P(r) file.



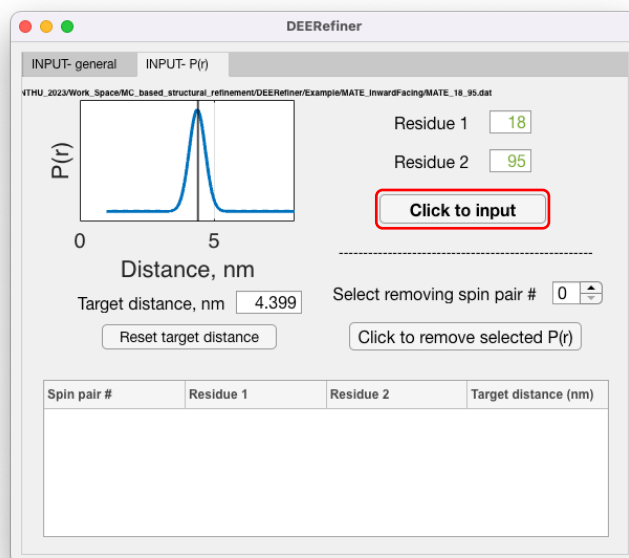
2. Selecting target peaks by left clicking your mouse.



3. Input corresponding residues of this distance distribution.



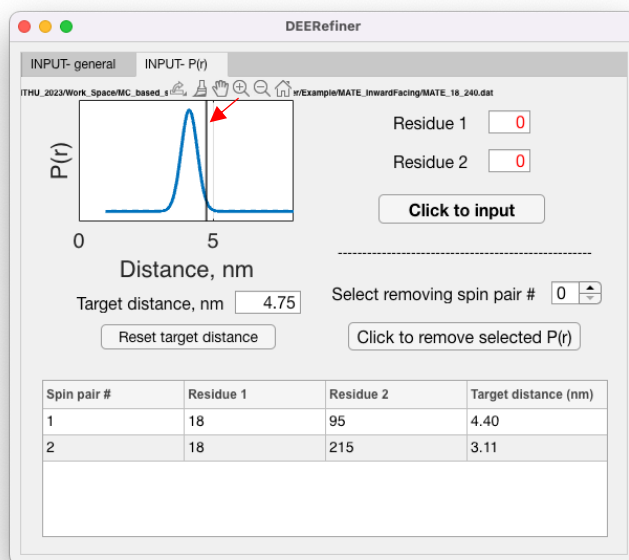
4. Input the data by clicking “Click to input”.



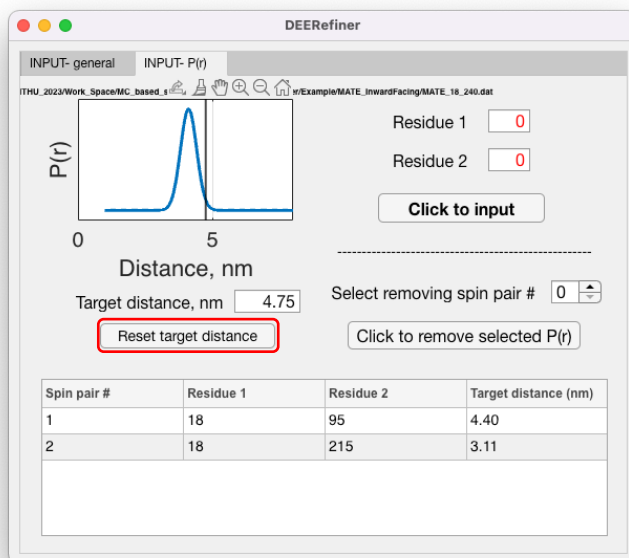
Step 3- Reselect target distance (optional)

Users can reset the target distance.

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



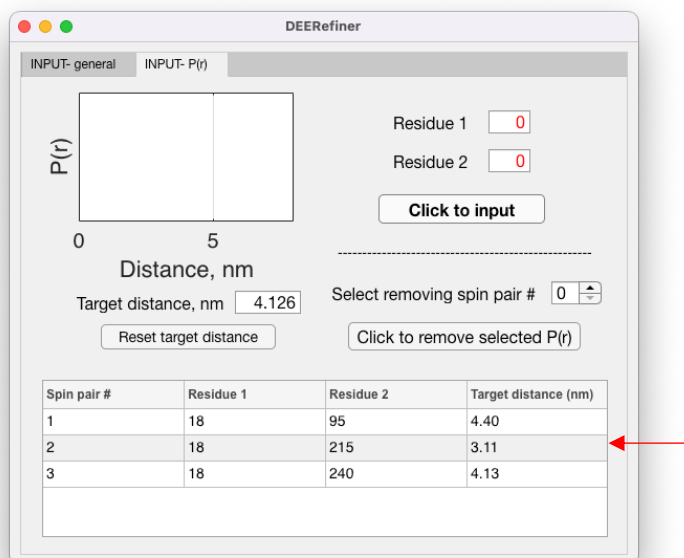
2. Reset the target by clicking “Reset target distance”.



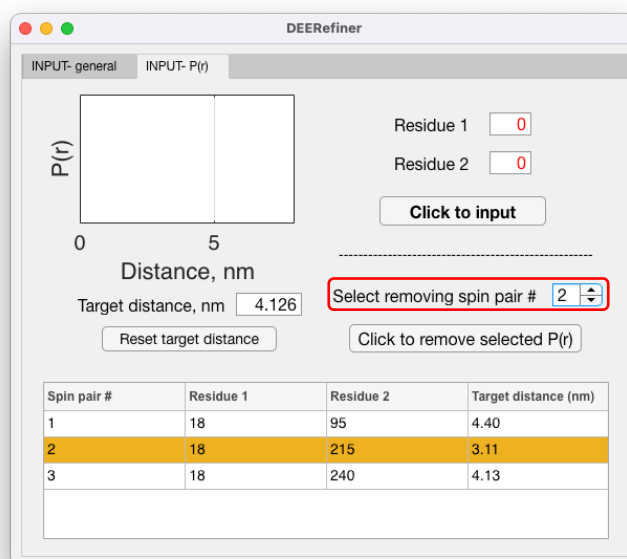
Step 4- Removing wrongly-loaded distance distribution files (optional)

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 $P(r)$ ”.

DEERefiner

INPUT- general INPUT- $P(r)$

$P(r)$

Distance, nm

Target distance, nm

Residue 1

Residue 2

Click to input

Select removing spin pair #

Reset target distance

Click to remove selected $P(r)$

Spin pair #	Residue 1	Residue 2	Target distance (nm)
1	18	95	4.40
2	18	240	4.13

Step 5- Setting parameters

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

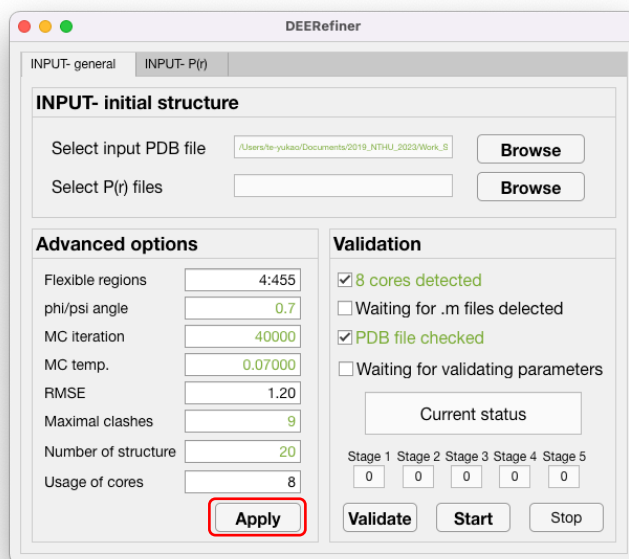
However, the definition of each parameter are listed below in case users want to change them manually.

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

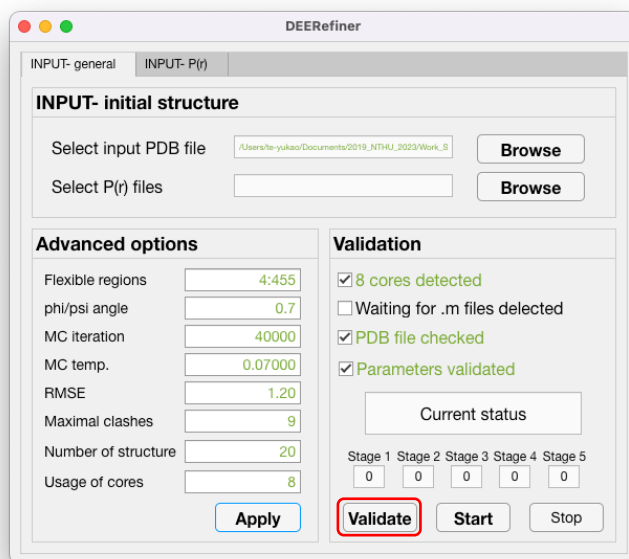
Option 1. Execute simulation with GUI Click the Start button.

1. Input parameters by clicking “Apply”.



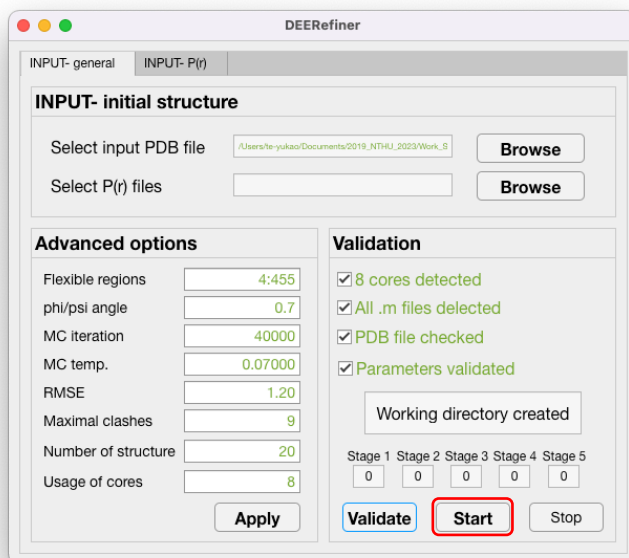
The image shows the DEERefiner GUI window. The 'INPUT- P(r)' tab is selected. Under 'INPUT- initial structure', the 'Select input PDB file' field contains a path and the 'Select P(r) files' field is empty. Both have 'Browse' buttons. The 'Advanced options' section has input fields for: Flexible regions (4:455), phi/psi angle (0.7), MC iteration (40000), MC temp. (0.07000), RMSE (1.20), Maximal clashes (9), Number of structure (20), and Usage of cores (8). The 'Apply' button at the bottom of this section is highlighted with a red box. The 'Validation' section shows: ☒ 8 cores detected, ☐ Waiting for .m files detected, ☒ PDB file checked, and ☐ Waiting for validating parameters. Below this is a 'Current status' button and a progress table with 5 stages, each showing a value of 0. At the bottom are 'Validate', 'Start', and 'Stop' buttons.

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



The image shows the DEERefiner GUI window after clicking 'Apply'. The 'Advanced options' section now has a blue 'Apply' button. In the 'Validation' section, a new checkbox ☒ Parameters validated has appeared. The 'Validate' button at the bottom is highlighted with a red box. All other elements, including the progress table and 'Start/Stop' buttons, remain the same as in the previous screenshot.

3. Execute simulations by clicking “Start”.



Option 2. Execute simulation with command line

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

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