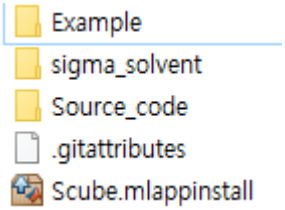
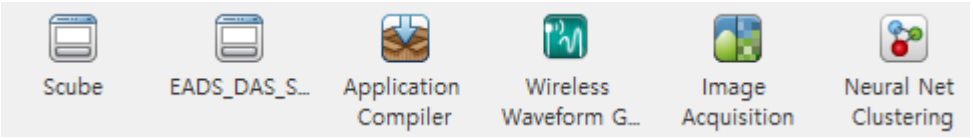
Read me for S-cube app

1. Installation.

Run Matlab.

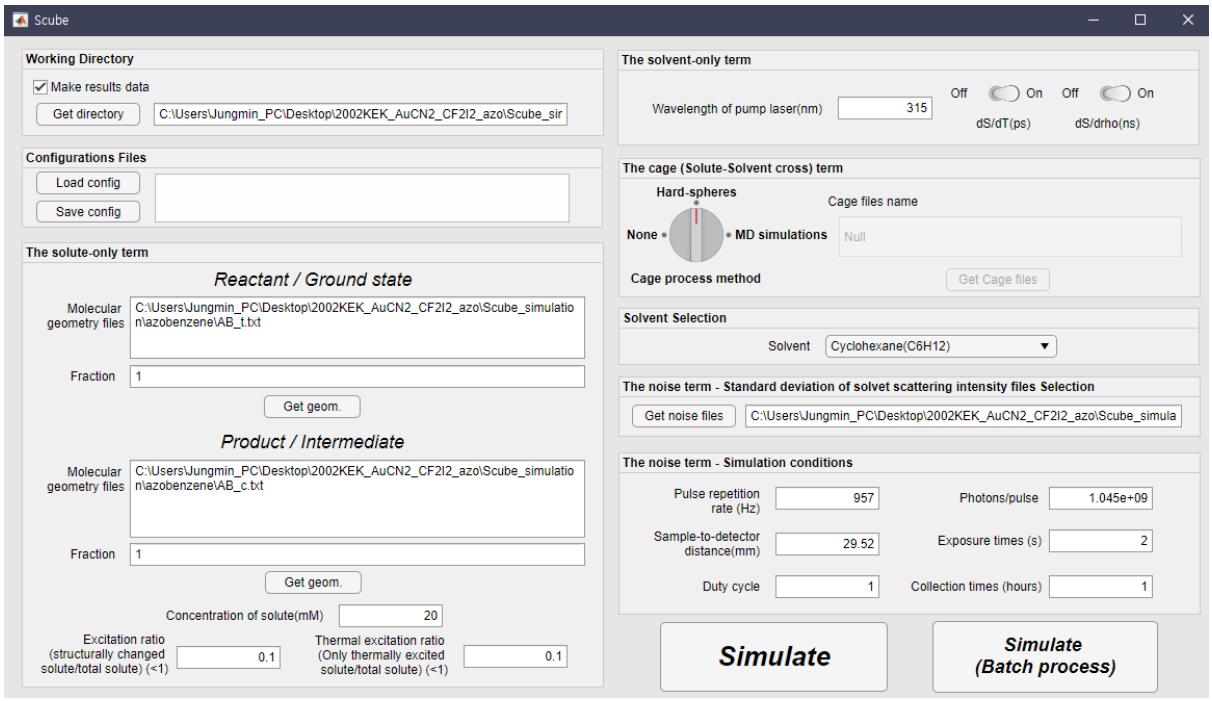


Run Scube.mlappinstall.



The Scube app is registered in your MATLAB apps library.

2. GUI Explanation



The values concentration of solute, excitation ratio, thermal excitation ratio, wavelength of pump laser, pulse repetition rate, photons/pulse, sample-to-detector distance, exposure times, duty cycle, collection times should be entered to simulate by referring paper.

Press the “Get directory” button to open the folder selection dialog box where you can set the working directory. The results file is created in the working directory.

You can load a configuration file by pressing the “Load config” button. Each simulation generates a configuration file. You can load a simulation by loading a configuration file. The example configuration file is “Example\config \Scube_config_190910_005600.dat”. You should rewrite the path to use the configuration file.

You can save the configuration file by pressing the “Save config” button.

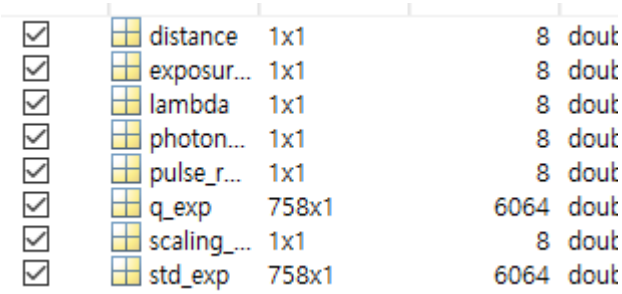
By pressing the “Get geom.” button you can set up a coordination file with a structure of reactant / ground state or product / excite state. Alternatively, you can enter the coordination files path directly in “Molecular geometry files”. The example file is “Example \ structure \ CHI2_Scube.txt”.

“Fraction” is the ratio of the excited structures. For example, 1 (for one coordination), [1,1] (for two coordination)

The switches of dS / dT and dS / drho can select whether to include the values of dS / dT and dS / drho in the simulation. If you select Off, the component are calculated as 0.

The cage process method knob can set the calculation method of the cage signal.If you select MD simulation, you need to insert the file that shows the q-S (q) value of the calculated MD simulation.

Pressing the “Get noise files” button opens a file selection window to select the experimental noise file to be referenced. The example is “sigma_solvent/cyclohexane_KEK.mat”.



The experimental noise file is a .mat (MATLAB variable) file consisting of the variables shown above.

Press the Simulate button to run the simulation. Simulation results are written under the working directory.

By pressing the Simulate batch button, you can read all the configuration files in the working directory and run a batch simulation.

3. How to make custom experimental noise file

An example is provided in the "Example\sigma_solvent_maker\cyclohexane_esrf.m" file.

```
clear all

solvent_data=dlmread('cyclohexane_esrf.dat');

q_exp=solvent_data(:,1);
std_exp=solvent_data(:,2);

clear solvent_data

pulse_repetition=1000; %Hz
exposure_time=1.5; %s
photons_per_pulse=5e8; % #photons/pulse
scaling_factor=3.35e+02; % Scaling one solvent molecule scattering intensity from detector to MD simulation.
distance=36.7; % mm
lambda=0.7187; % A

save sigma_cyclohexane_esrf;
```

Write the q, standard deviation of solvent scattering curves, pulse repetition rate, exposure time, photons per pulse, scaling factor, sample to detector distance, and X-ray wavelength of the experimental data to be used as a reference and run the code as shown above.