Tutorial for

Global Pathway Selection

Algorithm Package, Version 1.0.0

Prof. Wenting Sun's Group
Georgia Institute of Technology
Atlanta, GA, USA

Feb 2016

Global Pathway Selection (GPS) is an algorithm to effectively generate skeletal (reduced) mechanisms of complex chemistry mechanisms, developed by Prof. Wenting Sun's group at Georgia Institute of Technology. This document provides a tutorial to use this algorithm package with friendly user graphic interface.

How to cite:

X. Gao, S. Yang, W. Sun, "A global pathway selection algorithm for the reduction of detailed chemical kinetic mechanisms", Combustion and Flame, 2016

Contents

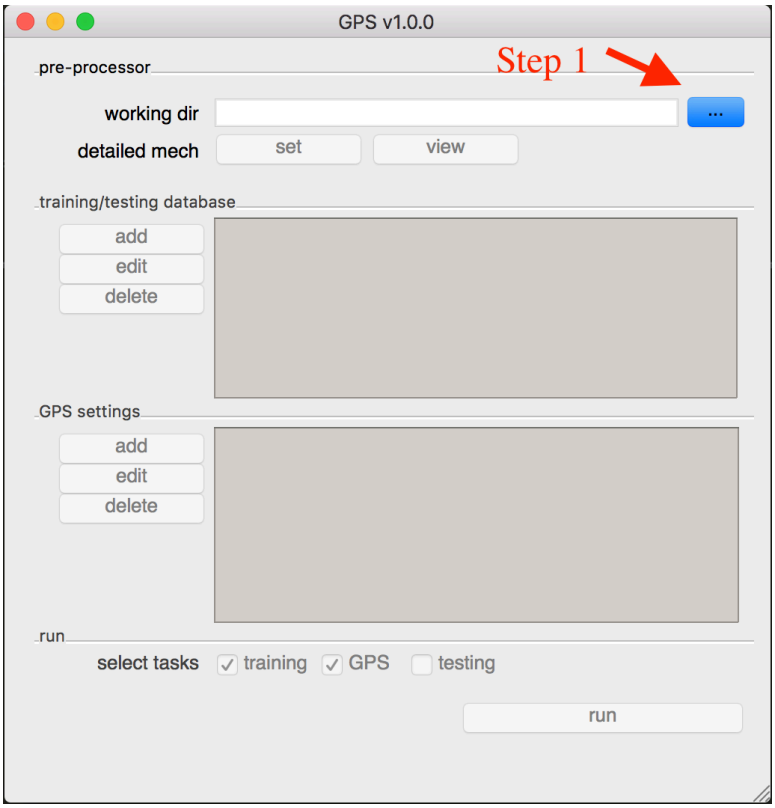
Steps

0. Download

You just need to download the executable file from our website (http://xianggao.weebly.com/gps.html)
Save it anywhere you want, and run it. There's no installation step.

1. Select the working directory

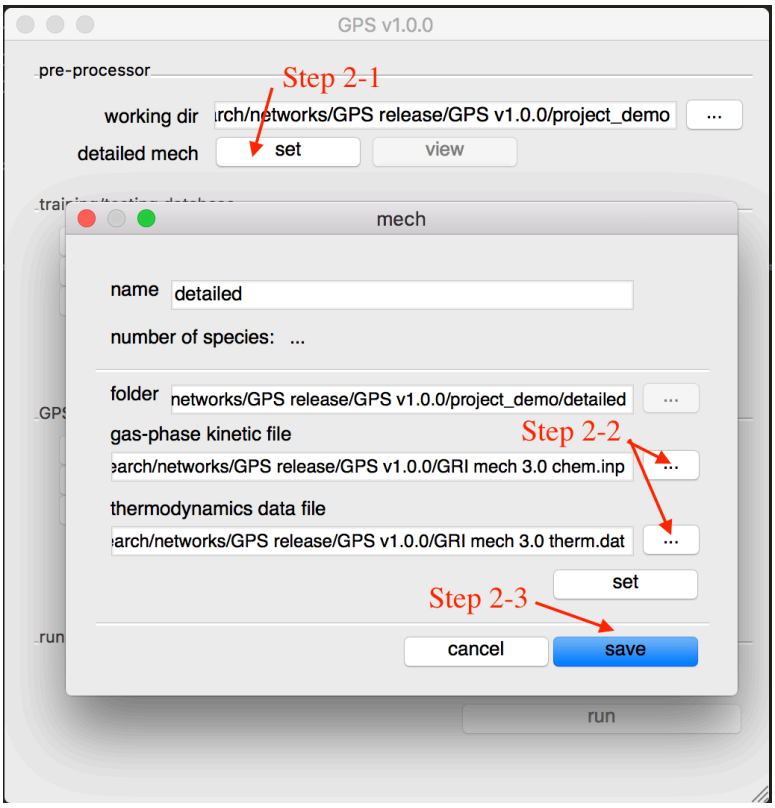
The first thing you need to do is to define your working directory (folder) with the button pointed by the red arrow in the figure below (Step1)



If this is a new project you want to start, we suggest you to create a new folder as your working directory. Assuming we created a folder "project_demo" for it.

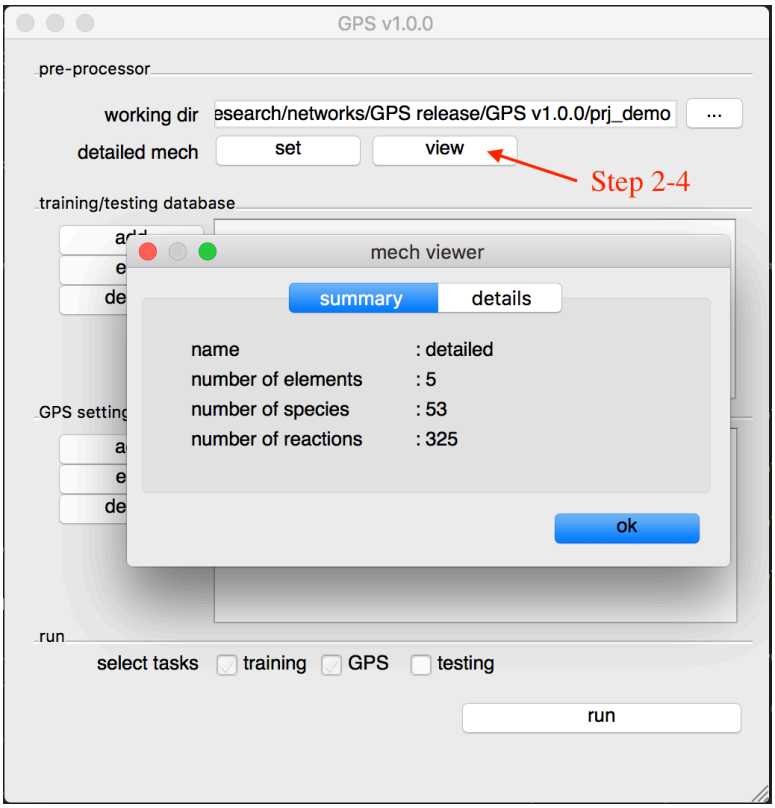
2. Set the detailed mechanism

The skeletal mechanism is generated from a detailed mechanism. So we need to define such detailed mechanism. To do this, you just need to click the button set (Step 2-1)



Then you will be prompted with a new dialog. You need to select the gas-phase kinetic file, and thermodynamics data file (Step 2-2). In this example, we chose GRI Mech 3.0.

Then you click save (Step 2-3). It may take seconds to read the mechanism files if they are large. After that the dialog will close automatically, which means the mechanism files are successfully processed.



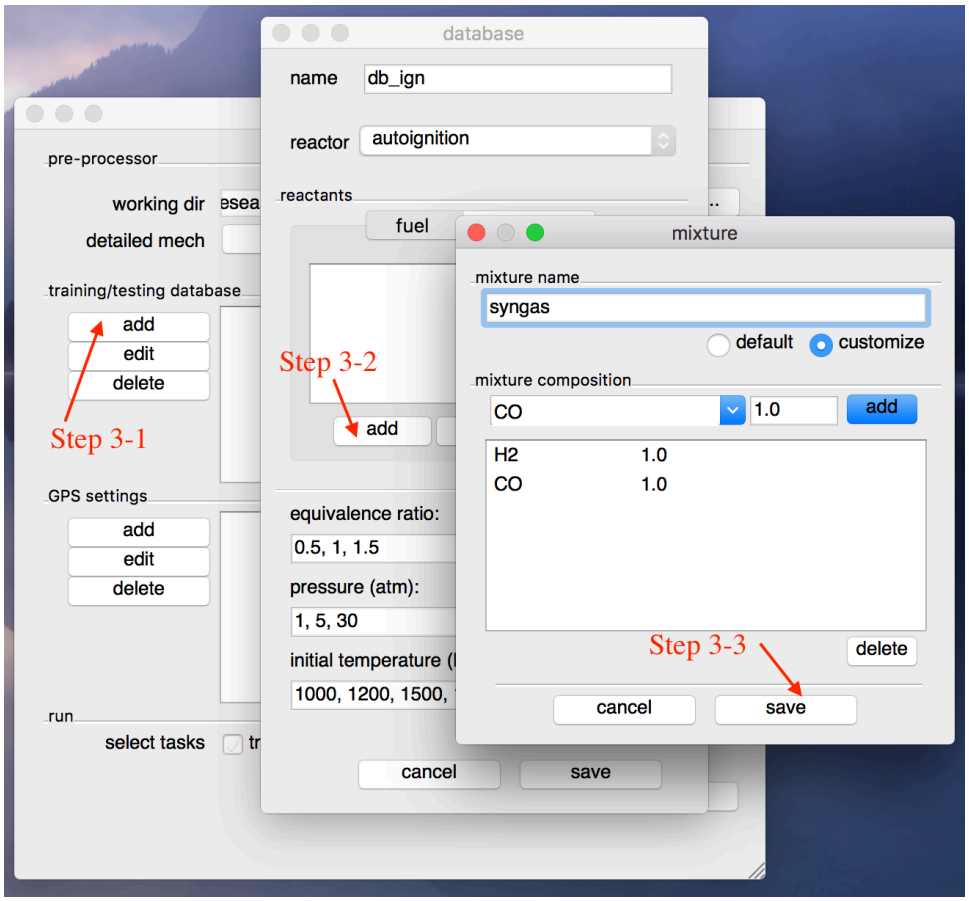
You now should be able to view the detailed mechanism you just defined (Step 2-4), and the new dialog will show you the number of elements, species, and reactions in the tab “summary”, and what they are in tab “details”

3. Define the database

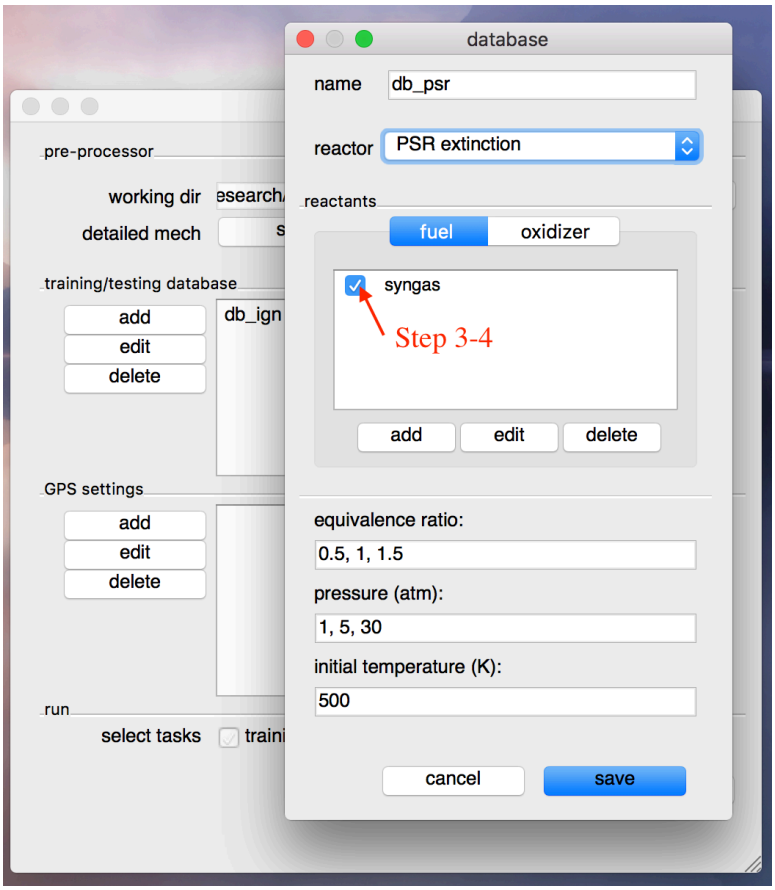
For GPS, the skeletal mechanism is obtained by analyzing the simulation results (the database) generated using the detailed mechanism. Therefore the next step is to define these databases.

You need to add a database by clicking the button “add” (Step 3-1), which gives you a new dialog “database”. You can give a name to this database, select what reactor you use (autoignition or PSR extinction), the equivalence ratios, pressures, and initial/inlet temperatures. For the reactants (fuel and oxidizer), you may need to add them manually (Step 3-2). In the dialog “mixture”, you can define the composition of this reactant (single component is fine) and give it a customized name (after choosing the “customize” radio button). Please save it (Step 3-3) and do the similar procedure for oxidizer.

In our example, we defined a H2/CO mixture as the fuel, with mole ratio of 1:1, and name of “syngas”. The database is named as “db_ign” and the reactor is “autoignition”



Once you have defined a reactant, you can use it when you are defining another database. For example, assuming after defining the “db_ign” database, we want to add another database “db_psr”, we can simply use the “syngas” reactant by clicking it (Step 3-4).

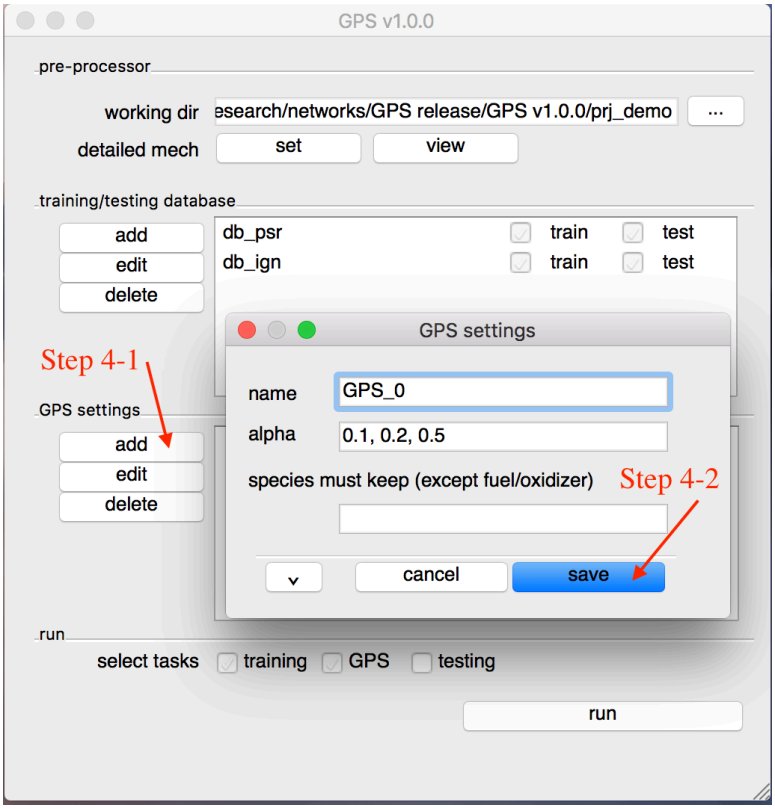


Usually we at least define two databases, one using “autoignition“ as the reactor, and another using “PSR extinction” as the reactor.

4. Define GPS settings

The idea behind GPS idea is basically to rank species by their (estimated) importance, then remove the species below a certain threshold value. This threshold value needs to be given by the user.

Therefore we need to create a GPS setting (Step 4-1). In the dialog you are prompted with, you can list the threshold values (alpha) you would like to try. Usually, the greater the alpha is, the smaller the obtained skeletal mechanism is, and the less this skeletal mechanism is. Please note that alpha should be a number between 0 and 1, and don't forget to save it (Step 4-2).



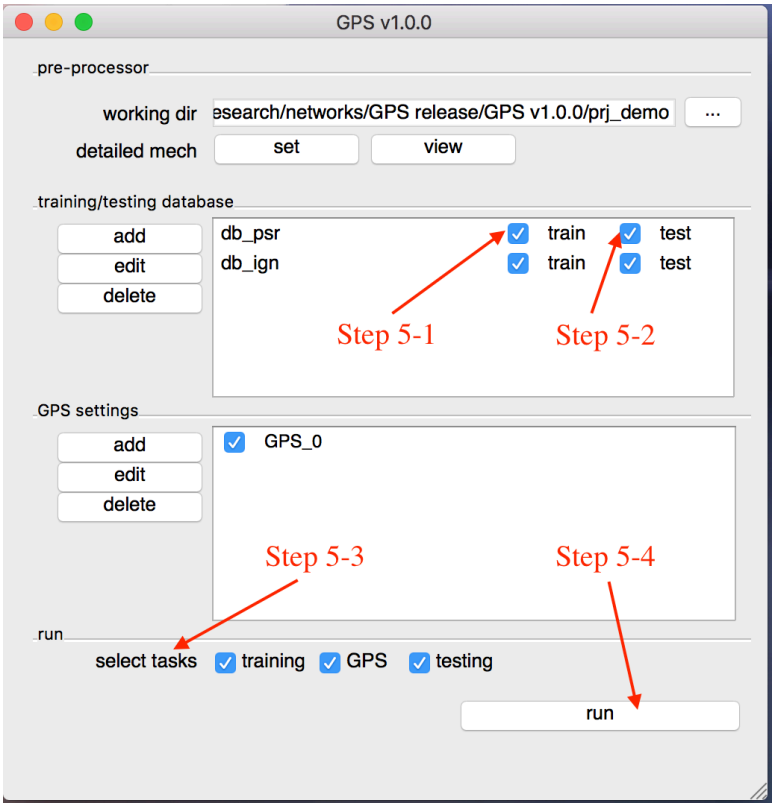
Actually, GPS has more than one parameter. However, to authors experience, usually only varying alpha is sufficient to generate all necessary candidate skeletal mechanisms.

5. Run

The final step is to select the tasks you want to run.

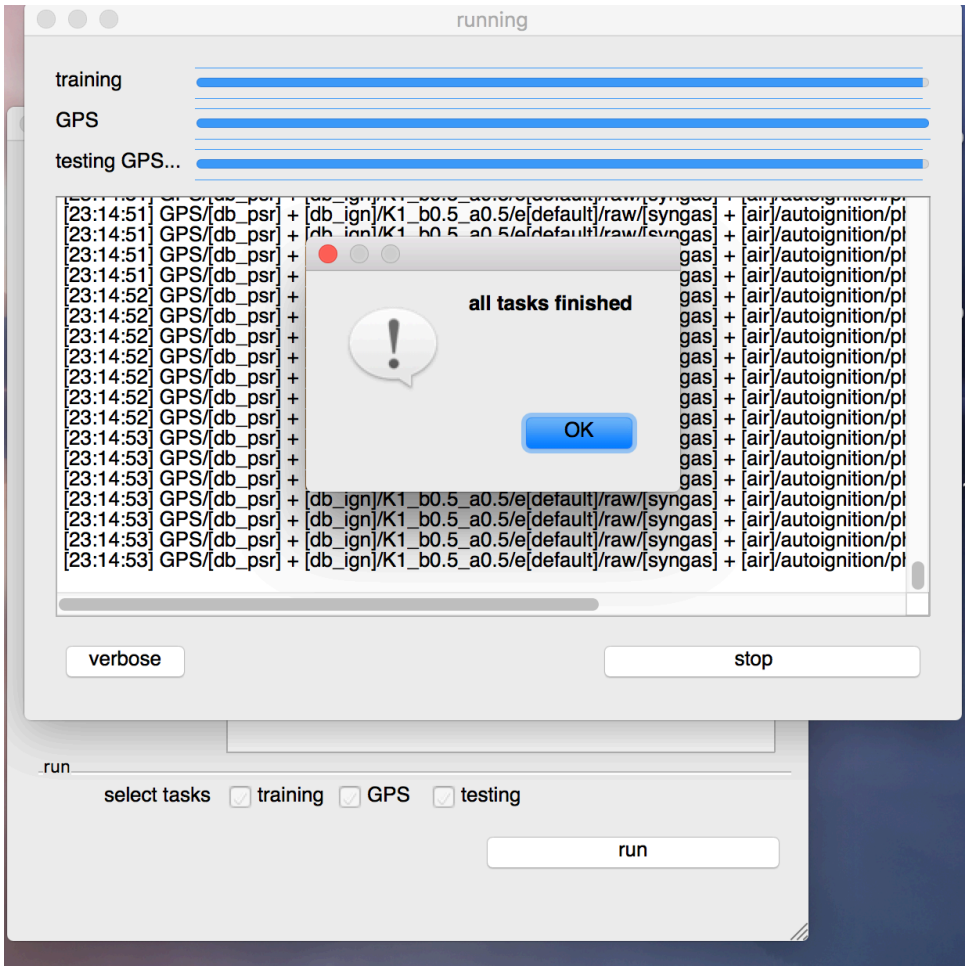
Firstly, you need to select what database you want GPS to consider when it generates the skeletal mechanism. You can click "train" for these databases (Step 5-1)

Usually, when we generate a skeletal mechanism, we want to test them to see how it behaves comparing the detailed mechanism. You can do this by simply clicking the databases you want to test on (Step 5-2).



Then you can choose the tasks (Step 5-3): "training" means only performing the simulations defined by databases using the detailed mechanism; "GPS" means performing GPS algorithm based on the training database; and "testing" means testing the skeletal mechanisms GPS generated on the testing database.

After this, you can run (Step 5-4). Progress will be shown in the progress bar below, and message box will be shown after all tasks have been finished.


running
training
GPS
testing GPS...
[23:14:51] GPS/[db_psr] + [db_ign]/K1_b0.5_a0.5/e[default]/raw/[syngas] + [air]/autoignition/pl
[23:14:52] GPS/[db_psr] + [db_ign]/K1_b0.5_a0.5/e[default]/raw/[syngas] + [air]/autoignition/pl
[23:14:53] GPS/[db_psr] + [db_ign]/K1_b0.5_a0.5/e[default]/raw/[syngas] + [air]/autoignition/pl
all tasks finished
OK
verbose
stop
run
select tasks
training
GPS
testing
run

6. Save and load the project

To save the project, you can choose “save” under the menu “project”, or simply use “Ctrl+S”
The project will be saved as “project.json” under your working directory.

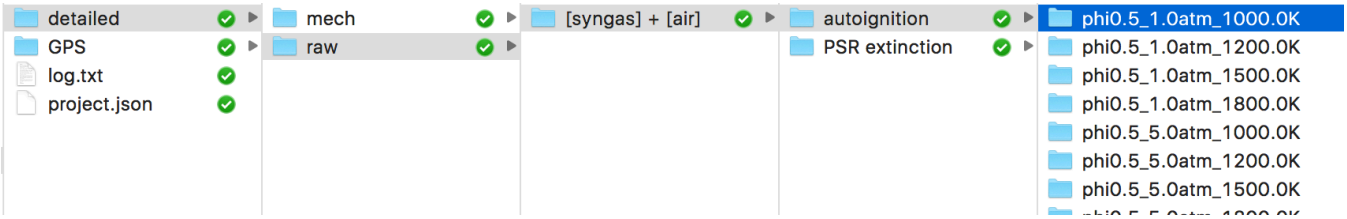
To load the project, you just need to choose the folder of this project as your working directory.

Output files

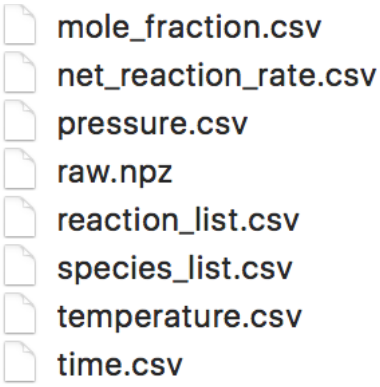
Training simulation results
The training simulation results will be stored in the folder

[working dir]/detailed/raw/[fuel]+[oxidizer]/reactor/[phi, atm, K]

For example, the folder highlighted in the figure below stores the simulation results of autoignition, using syngas as fuel, air as oxidizer, at equivalence ratio of 0.5, 1atm, and 1000K as initial temperature.



The simulation results will be several comma-separated files (.csv)



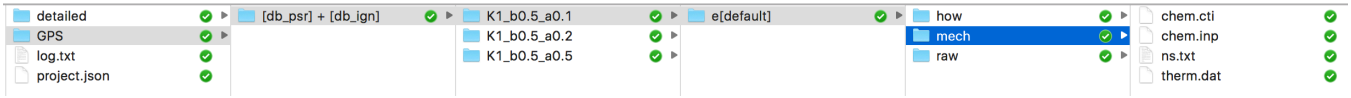
Where the unit for net reaction rate is mole/m^3-s, for pressure is atm, for temperature is K, and for time is s. For net reaction rate, and mole fraction, each row corresponds to a time point in time.csv, each column corresponds to a species or a reaction, with same order as in species_list.csv or reaction_list.csv

If you define "ignition" as the point where the temperature is greater than the initial temperature by 400K, the last value in time.csv will be the ignition delay.

Skeletal mechanisms

The obtained skeletal mechanisms will be stored in the folder
[working dir]/GPS/[training database]/[GPS parameters]/[element parameters]/[mech]

These include chem.inp and therm.dat
The number of species can be found in ns.txt or in chem.inp



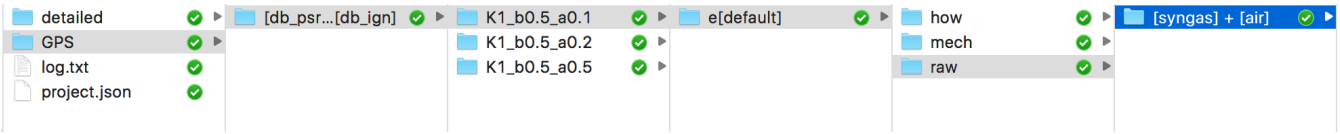
"K1_b0.5_a0.1" means alpha value is 0.1 ("a" stands for "alpha" here).

Testing simulation results

The testing simulation results (which are obtained using GPS skeletal mechanisms) will be stored in the folder

[working dir]/GPS/[training database]/[GPS parameters]/[element parameters]/[raw]/[fuel]+[oxidizer]/reactor/[phi, atm, K]

For example, as highlighted in the folder shown below.



"K1_b0.5_a0.1" means alpha value is 0.1 ("a" stands for "alpha" here).