

## How to use software?

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Note: These directions are how to use the entire software package, but I am currently not releasing the createhardcode program, only releasing the hardcoded output that can be used to run simulations under the GNU general purpose license.

### Matlab/Octave:

- The mechanism you want to use should be named chem.inp
- chem.inp should have all thermodynamic data in the file, do not use a separate therm.dat file  
(if using Octave version make sure all blank lines are removed)
- Run createhardcode.m
- A folder "hardcode" will be created
- You may have to change the fuel species in the reactor file to match your mechanism for instance changing "CH4" to "H2"
- simply run reactor the reactor .m file in matlab

Note: to use the reactor\_3dplotcode.m file, you must have the matlab parallel computing package installed and a verified cluster profile. You can click on Parallel>>Manage Cluster Profiles>>Verify

### Octave-Fortran hybrid version:

- The mechanism you want to use should be named chem.inp
- chem.inp should have all thermodynamic data in the file, do not use a separate therm.dat file
- Run createhardcode.m
- A file mechsspecific.f will be created

- you may have to change the fuel species and also the length of NEQ and KK vectors in the RES function (DASSL solver has some glitches when trying to pass a variable containing these vector lengths)
- you must run the run\_reactor.....m file from octave, then plotoutput.m from octave

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