File Overview and Case Setup in CONVERGE Studio

CONVERGE Studio Workflow

- ***Case Setup* module**
  - Begin a project
  - Import the surface geometry
  - Prepare the surface
  - **Configure case setup**
  - Export input and data files to the Case Directory

--Run CONVERGE simulation--

- *Line Plotting* module

- *Post-Processing 3D* module

CONVERGE Workflow

CAD IMPORT+CLEAN

A **B** *.stl
—or—
A surface.dat

A	ASCII
FILE TYPE **B**	BINARY

ANALYSIS SETUP

A surface.dat
A *.in
A *.dat

CASE DIRECTORY

SOLVE IN CONVERGE

A *.echo
A **B** restart*.rst
A *.out
B post*.out

CASE DIRECTORY

VISUALIZATION

A *.out
B post*.out

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Input Files (1/2)

- All simulations require the following *.in* files
    - ○ **boundary.in**: Define boundary conditions
    - ○ **initialize.in**: Define initial conditions in the computational domain
    - ○ **inputs.in**: Define the grid size, activate models or other options, configure timing, etc.
    - ○ **post.in**: Specify how the 3D output will be written
    - ○ **solver.in**: Set up the PISO algorithm, transport equations, and linear systems

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Input Files (2/2)

- You may need additional input files such as *spray.in* for spray models or *turbulence.in* for turbulence model

- Create and edit input files, which are in ASCII format, in CONVERGE Studio (recommended) or a text editor

- Export all required input files into the *Case Directory* before running a simulation

Data Files (1/2)

- Simulations may require some of the following *.dat* files
  - o *surface.dat*: Information on surface triangulation and boundary IDs (always required)
  - o *mech.dat*: List of elements and species and, if applicable, reaction data
  - o *therm.dat*: Species-specific thermodynamic data
  - o *gas.dat*: Gas properties, such as viscosity and conductivity, as a function of temperature
  - o *liquid.dat*: Liquid properties, such as viscosity and vapor pressure, as a function of temperature
  - o *solid.dat*: Solid properties, such as density and conductivity, as a function of temperature
  - o *transport.dat*: Coefficients to calculate mixture-averaged diffusion, conductivity, and viscosity
  - o *surface_mech.dat*: Information on surface species and their reaction mechanisms
  - o *surface_therm.dat*: Thermodynamic information for surface species

Data Files (2/2)

- For data files such as *gas.dat, liquid.dat,* or *solid.dat*, CONVERGE Studio contains a library of materials data from which it can create some of these **.dat* files

- We do not recommend manually editing the data files

- Export all required data files into the *Case Directory* before running a simulation

Surface Geometry File

- The surface geometry file (*e.g., surface.dat*) is required for all CONVERGE simulations

- You can edit the surface geometry in CONVERGE Studio and export the *surface.dat* file

- This file is used by the CONVERGE solver to automatically create the mesh at runtime

- Small changes in the geometry only requires changes to be made to *surface.dat* before running a new simulation

Thermodynamic Data File (1/2)

- The thermodynamic data file (*e.g., therm.dat*) only lists gas thermodynamic properties

- The file includes the chemical composition of each species and coefficients to calculate entropy and enthalpy at a minimum and a maximum temperature

```
THERMO
   300.000  1000.000  5000.000
AR                120186AR  1                  G   300.000  5000.000  1000.0          1
 0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-0.07453750E+04 0.04366000E+02 0.02500000E+02 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-0.07453750E+04 0.04366000E+02                   4
H               8/12/99 THERMH   1O   0    0    0G   300.000  5000.000 1000.000          1
 2.50104422E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 2.54747466E+04-4.65341317E-01 2.50104422E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 2.54747466E+04-4.65341317E-01                   4
```

Thermodynamic Data File (2/2)

- If there are two species with the same name, CONVERGE v2.3 uses the first entry

- CONVERGE Studio v2.3 warns of duplicates and lets you decide how to resolve them
  - Keep the 1st instance of each duplicate
  - Keep the last instance of each duplicate
  - Custom (pick manually)

- You can also choose to comment out duplicate lines without removing them permanently
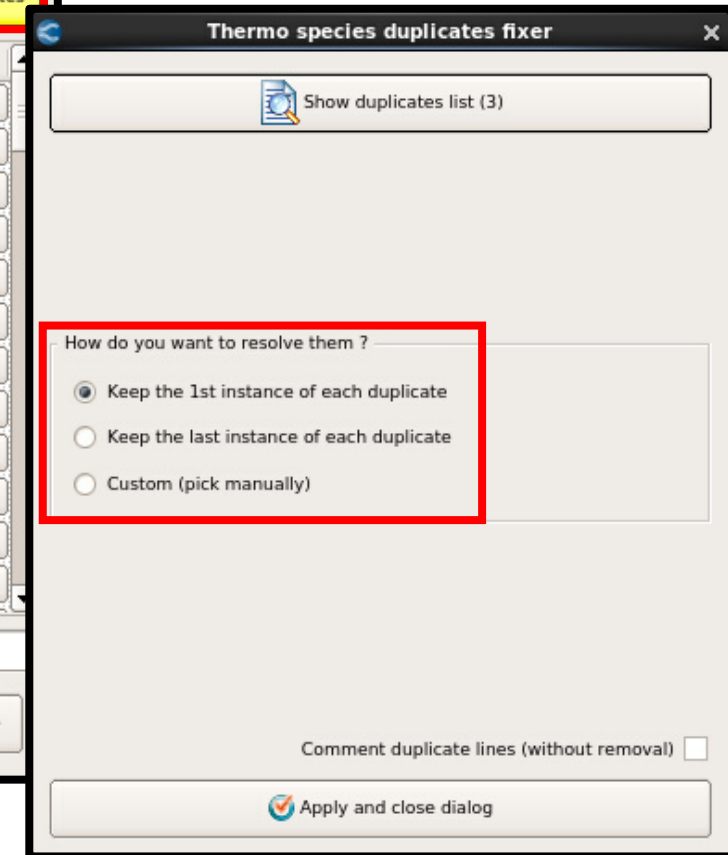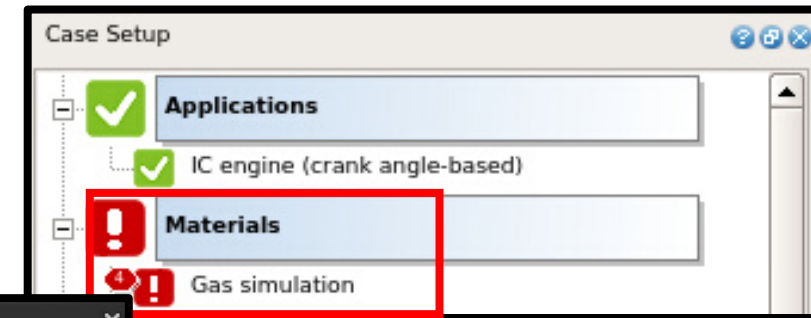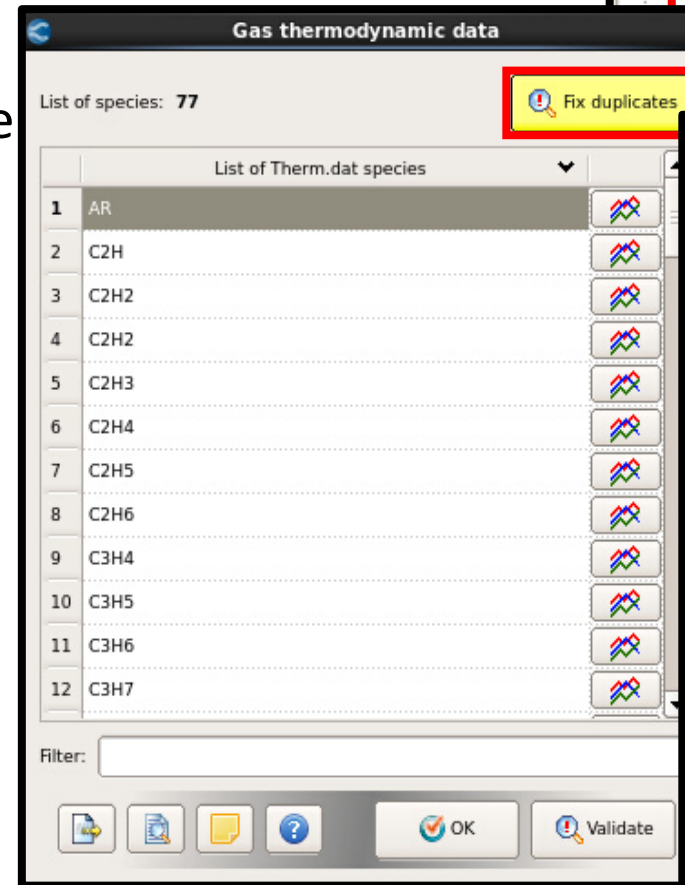
How to Set Up Input Files

- When setting up a case, it is more efficient to modify preconfigured input and data files than to begin with none

- There are two ways to use preconfigured files in the *Case Setup* module
  - Select a template in the main *Case Setup* dialog box
  - Import existing input and data files

- Use the *Case Setup* module to make modifications

Use a *Case Setup* Template

- Templates contain input and data files for selected types of simulations (*e.g.,* premixed combustion)

- The templates lack a *surface.dat* file

- You can load a template through the *Tools* menu or the *Case Setup* dock
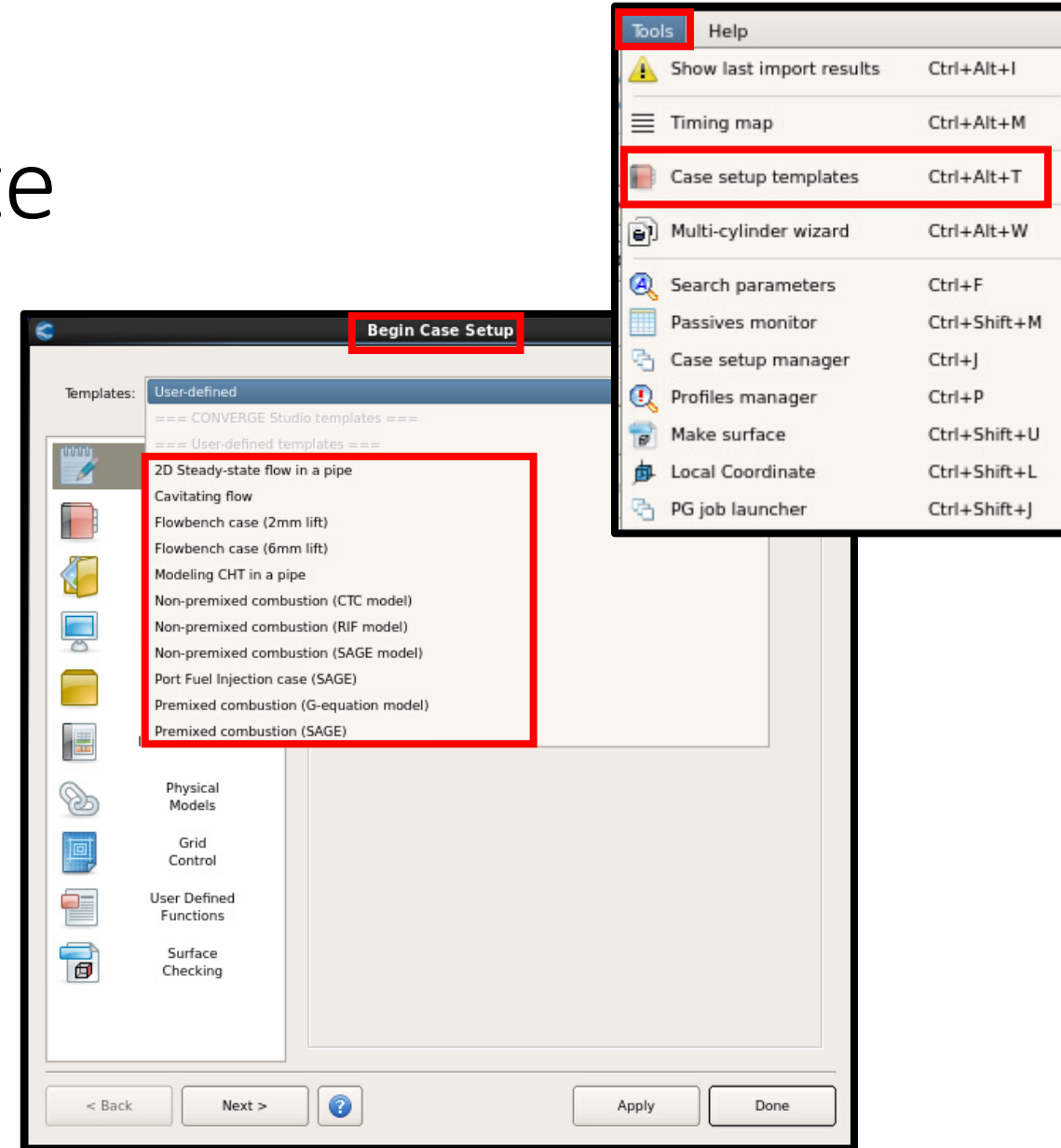
Import Existing Input and Data Files (1/3)

- You can import files into CONVERGE Studio in two ways

  o Go to *File > Import > Import input file(s)*

  o Click the <u>Import</u> button on the main toolbar
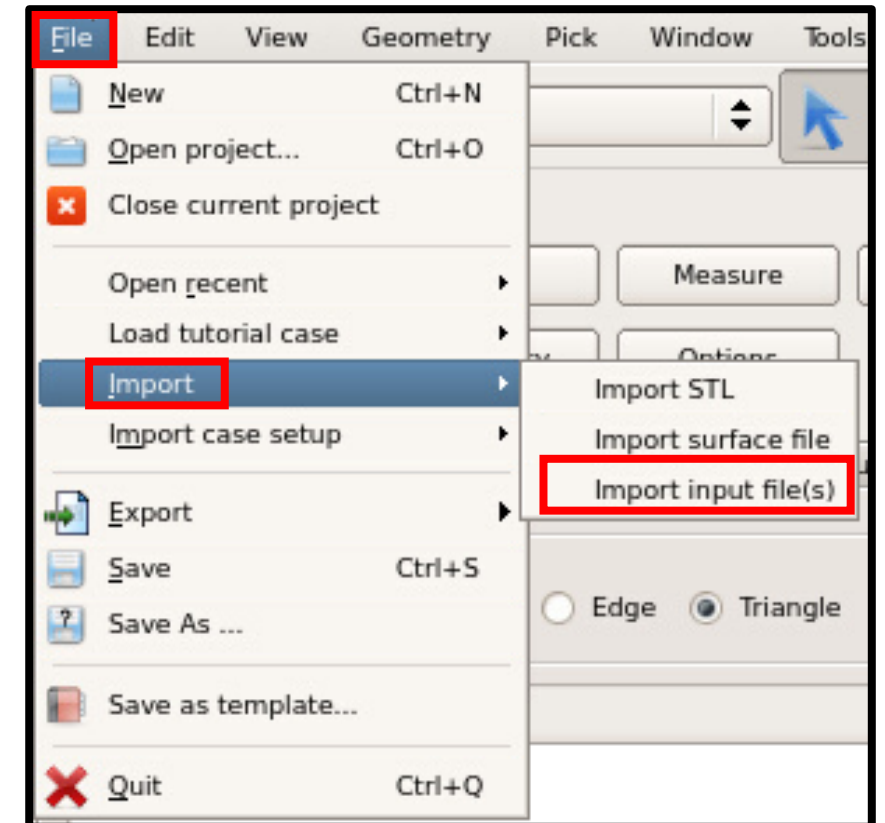
# Import Existing Input and Data Files (2/3)

- When you import input files from a previous version of CONVERGE, select the version in the drop-down menu

- If you click <u>OK</u>, CONVERGE Studio reads the format of all files to make them compatible with v2.3
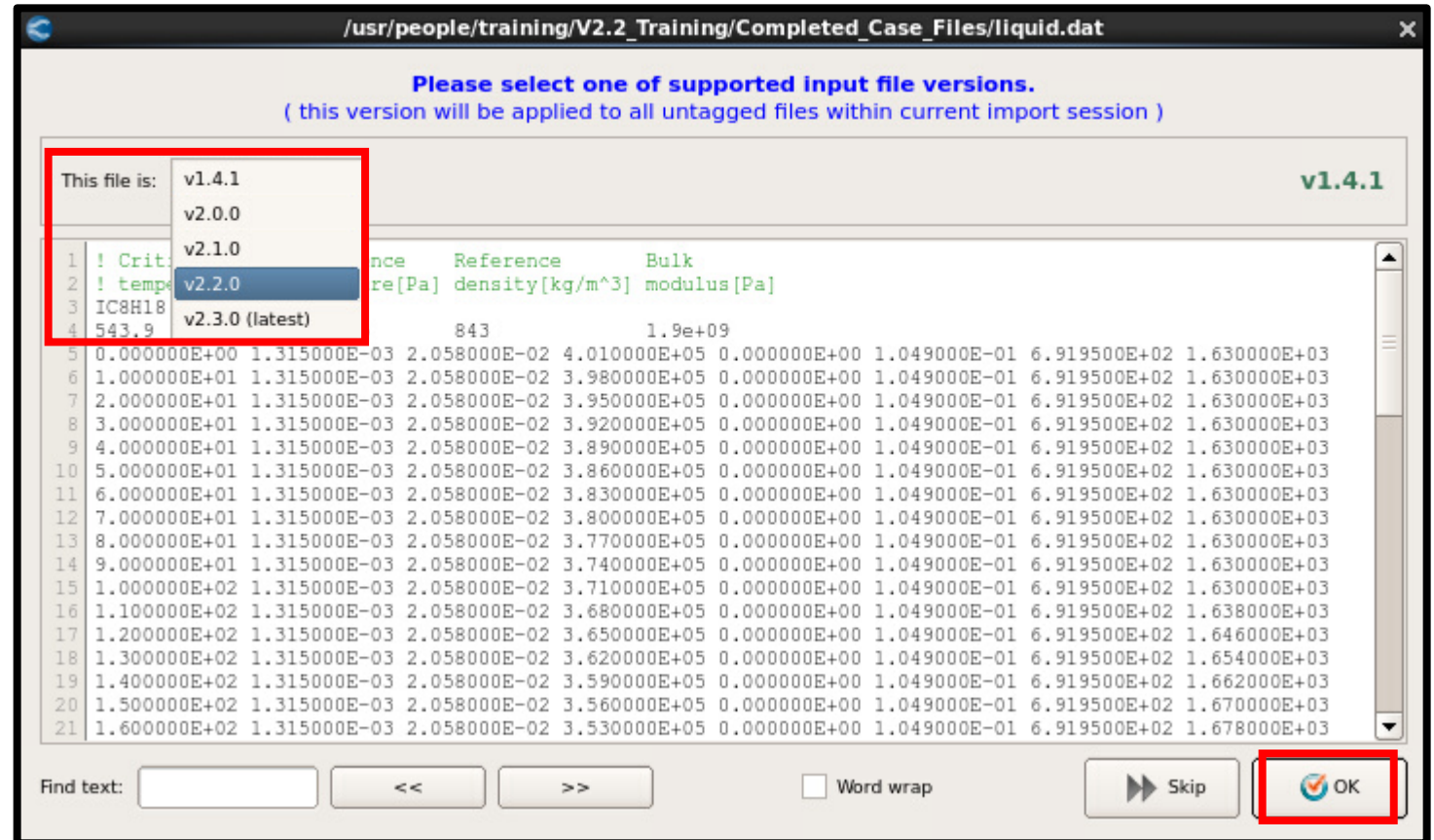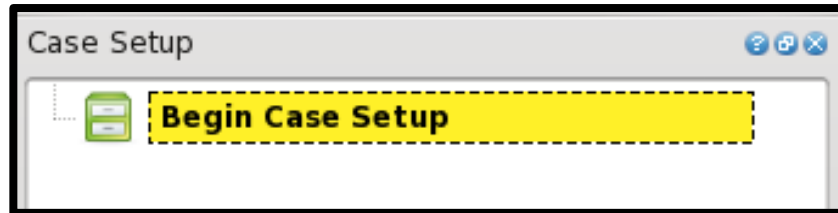
Import Existing Input and Data Files (3/3)

- A pop-up window and the *Import log* will show the results of the import, including any errors or warnings
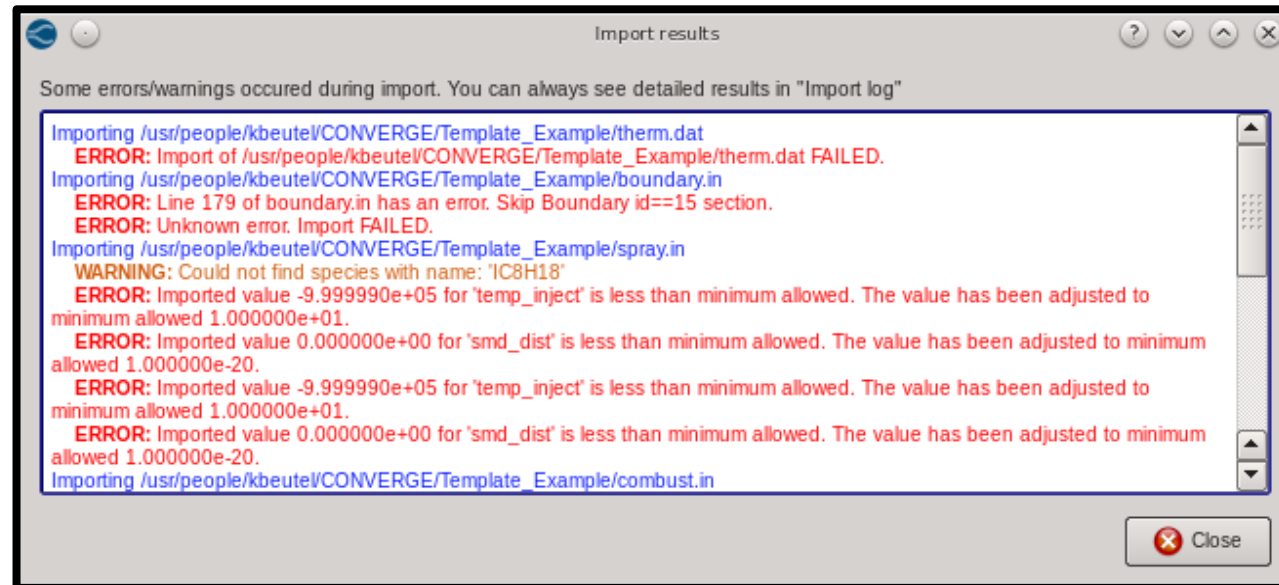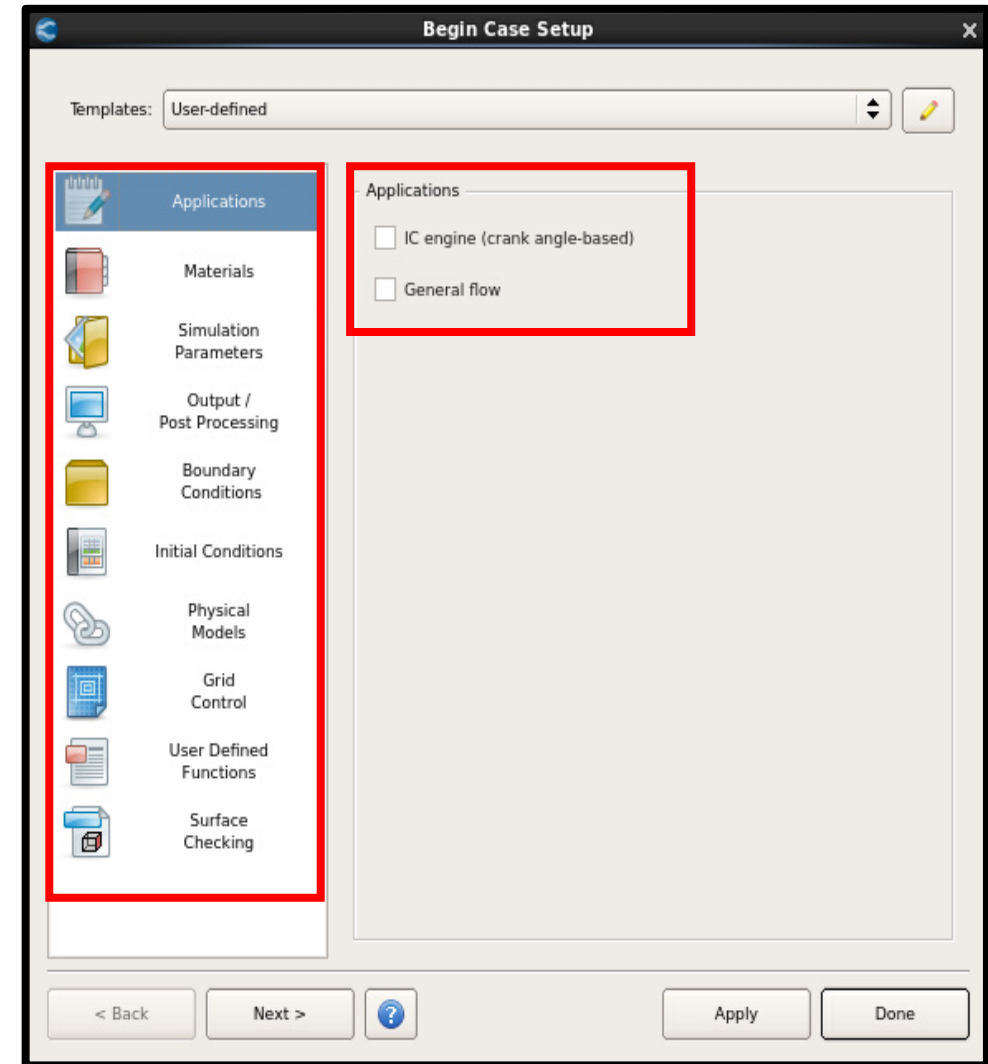

- After closing the pop-up window, you can still see this information in the *Import log*

Set Up New Input Files (1/3)

1) Go to the *Case Setup* dock and click <u>Begin Case Setup</u>

2) Click through the category list and check the relevant boxes

3) Click <u>Apply</u> or <u>Done</u>

Set Up New Input Files (2/3)

4) Click on a category in the *Case Setup* dock to open the associated dialog box

5) Fill in the required parameters in the dialog box

   • You can use the <u>Set recommended values</u> button

6) Click on the [icon] button to preview the input file
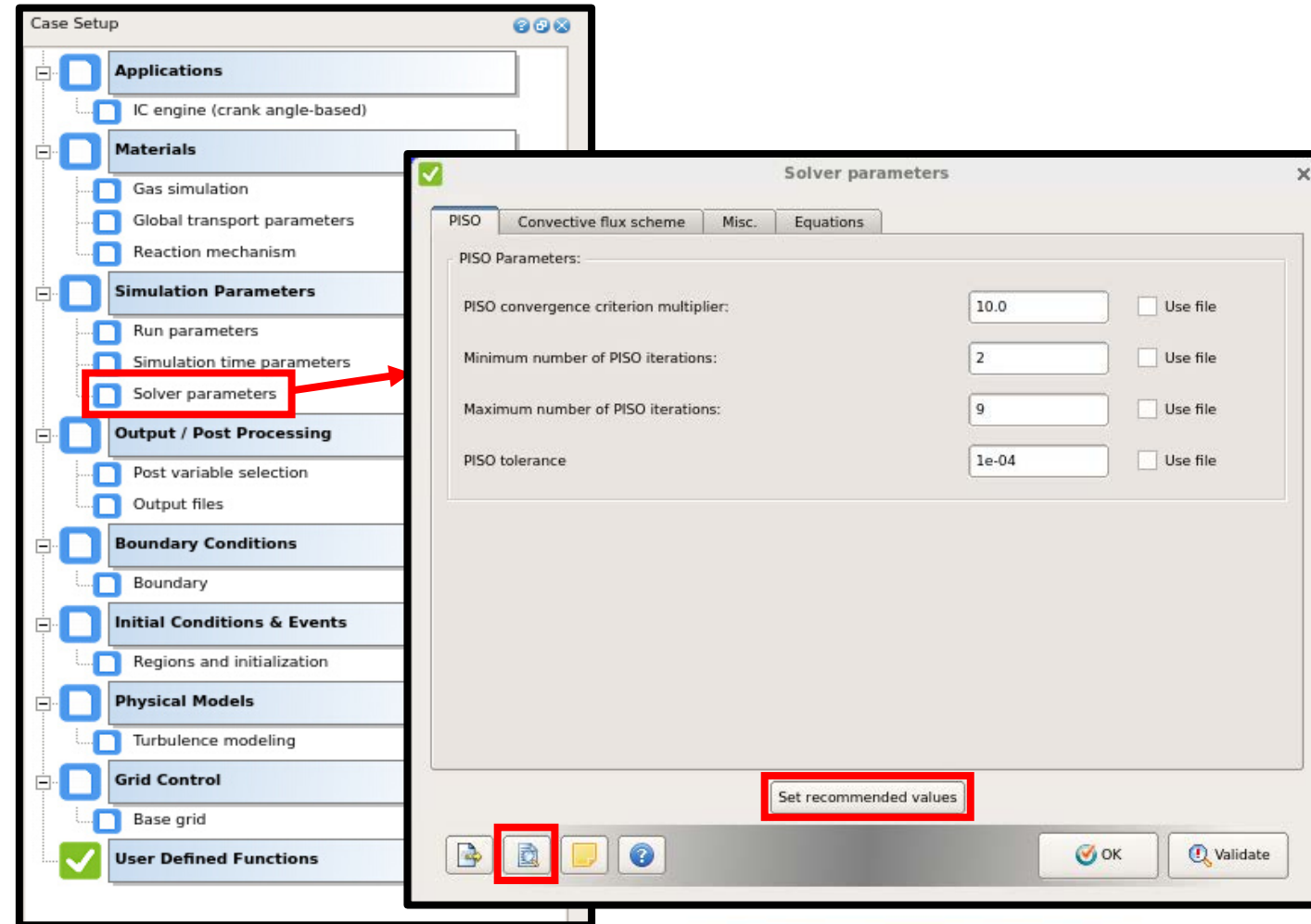
Set Up New Input Files (3/3)

- A warning ( ) or an error ( ) appears if the dialog box is not filled in correctly or completely

- Reopen the dialog box to fix the issue, generally highlighted in pink

- When all categories have a green checkbox, you are finished
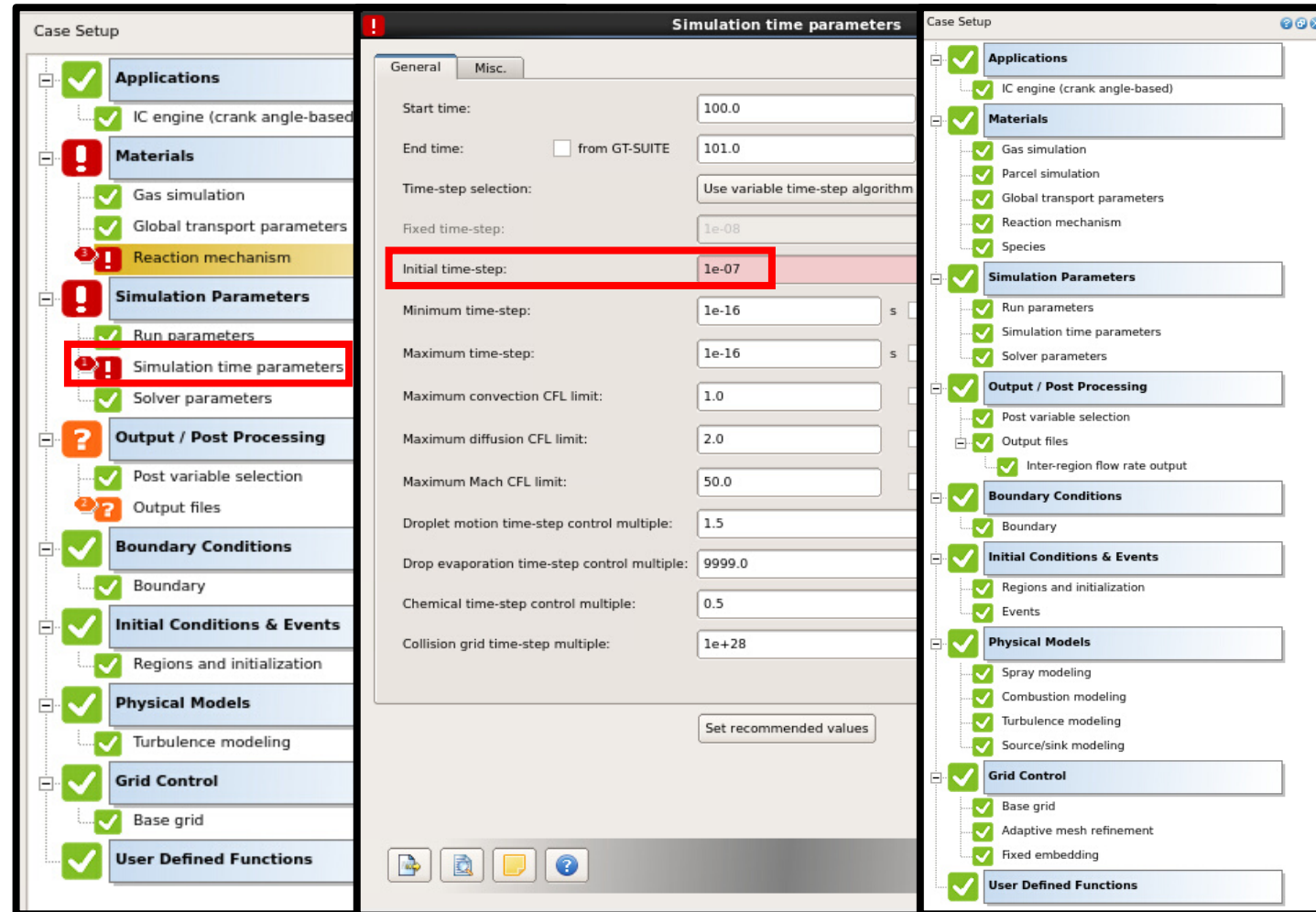
Editing Input Files While Running a Simulation

- You can change some input files while CONVERGE is running the simulation
  - These files include *inputs.in, solver.in,* and *amr.in* (maximum and minimum grid number and number of AMR cycles)
- To set CONVERGE to reread these input files at each time-step
  - Go to *Case Setup > Run parameters > Misc*
  - Check <u>Reread Inputs.in each time-step</u>
  - Click <u>OK</u>
- Before CONVERGE can read the changes made to the input files, you must save and export the files to the *Case Directory*

Output Files from CONVERGE

- The CONVERGE solver generates several types of output files while running a simulation
  - CONVERGE writes an *.echo* file for each *.in* file (*e.g., combust.in* will yield *combust.echo*) so you can verify that the inputs have been correctly read
  - CONVERGE writes restart files (*restart*.rst*) at a user-specified frequency
  - CONVERGE writes *.out* files (*e.g., thermo.out*), which contain spatially averaged or integrated quantities
    - The *post*.out* files contain individual cell quantities for all cells in the domain

THANK YOU!

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