

# ***Connecting Cantera and FLUENT***

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**Cantera Workshop  
30<sup>th</sup> Symposium on Combustion, July 2004**

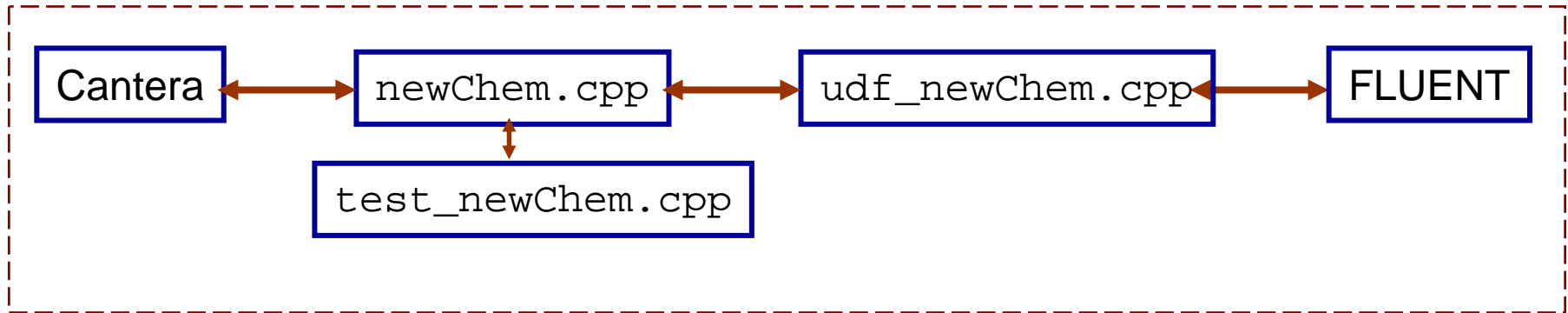
**The National Energy Technology Laboratory**



# Design of the Interface

## Design:

- mimic “Cantera-clib” interface
- The FLUENT udf-functions have no explicit reference to Cantera



## Why:

- interference between FLUENT and Cantera functions (Cvode)
- offline testing and debugging
  - be careful of memory leaks ( “ccmalloc” )
- functions can be used with other packages



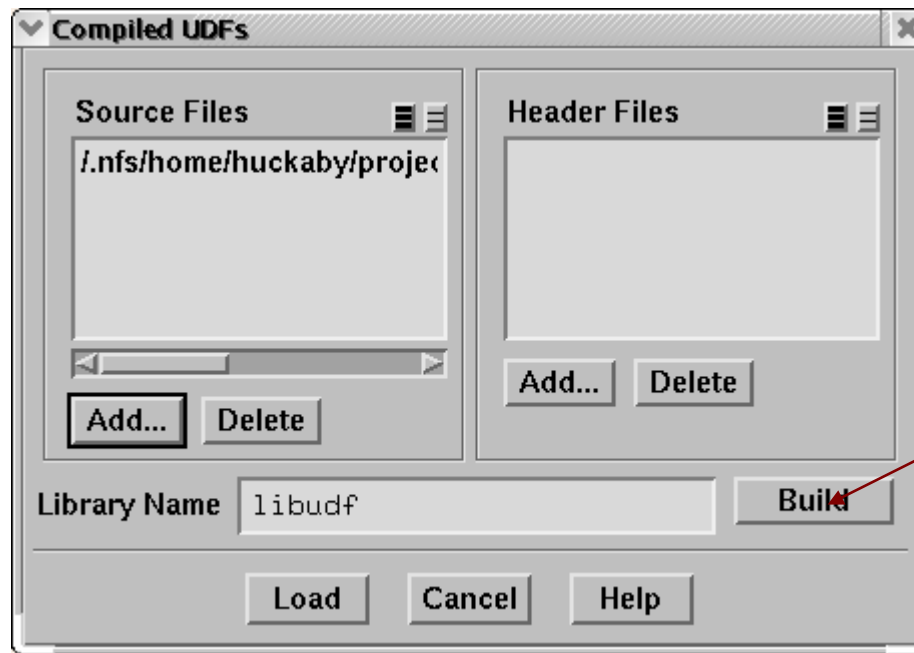
# Steps to connect FLUENT and Cantera

1. Create `libudf` directories structure
2. Create functions to manipulate Cantera objects ( `newChem.cpp`, `newChem.hpp` )
3. Test functions ( `test_newChem.cpp` )
4. Modify `libudf/Makefile`
5. Modify `libudf/src/makefile`
6. Create “hooks” between FLUENT and functions ( `udf_newChem.c` )
7. Manually compile sources
8. Load `udf_newChem` into FLUENT
9. Execute udf's



# Create libudf directory structure

1. Create empty file named `udf_newChem.c`
2. Define/user-defined/compiled – build button
3. This will create the structure and “makefiles” on the next page



# libudf Directory Structure

file:/nfs/home/huckaby/projects/cantera/fluent\_example - Konqueror

Location: file:/nfs/home/huckaby/projects/cantera/fluent\_example

Name	Size	File Type
GAMBIT.20630	4.0 KB	Directory
libudf		Directory
Inx86	4.0 KB	Directory
2ddp	4.0 KB	Directory
src	4.0	./libudf/src/makefile
makefile	5.9 KB	Makefile
makefile.bck	5.9 KB	Makefile
newChem.cpp	3.4 KB	C++ Source File
newChem.h	147 B	C Header File
testNewChem.cpp	629 B	./libudf/Makefile
udf_names.c	804 B	C Source File
udf_newChem.c	2.8 KB	C Source File
udf_newChem.c.bck	2.1 KB	C Source File
Makefile	1,005 B	Makefile

49 Items - 43 Files (3.7 MB Total) - 6 Directories



# Create functions which access Cantera newChem.cpp

- Create in libudf/src
  - contains objects to access Cantera functionality
  - extern "C" { ... to "de-mangle" c++ functions

```
static Cantera::IdealGasMix *_gas;  
static vector<int> _speciesMap;  
static vector<int> _speciesMapInv;  
static vector<double> _massFractions;  
static int _nCantera = 0;  
static int _nFluent = 0;  
static Cantera::ChemEquil *_equil;  
  
extern "C" {
```



# Create a header file for functions newChem.h

- Create in libudf/src

```
void newChem_newChem( const int nFluent );  
void newChem_addToMap( const int fluent_index, const char *name);  
void newChem_equil_HP(double *T, double *p, double Y[]);
```

- Extern "C" is not needed
- Three functions
  - Initialization
  - map between species indices
  - equilibrate the composition



# Test the newly created functions

- Create a directory test
  - Create/Edit Makefile (look at `cxx_examples`)

```
CANTERA = /nfs/home/huckaby/projects/cantera/cantera_dev
CANTERA_INC = $(CANTERA)/include/cantera
CANTERA_LIB = -L$(CANTERA)/lib/cantera/1.5.4 \
-lzeroD -ltransport -lconverters -lcantera -lrecipes \
-lcvsode -lctlapack -lctmath -lctblas -ltpx -lctcxx \
-L/usr/lib/gcc-lib/i386-redhat-linux/2.96 -lg2c -lstdc++\
-lgcc -lm
```

```
CXX = g++
CXX_FLAGS = -g -O
CXX_INC = $(CANTERA_INC)
```





## Makefile cont'd

```
default: test.exe

newChem.o: ../libudf/src/newChem.cpp
    echo $(CANTERA_INC)
    g++ -g -c -I$(CANTERA_INC) -I/usr/include/g++
    ../libudf/src/newChem.cpp

testNewChem.o: testNewChem.cpp
    g++ -g -c -I$(CANTERA_INC) -I../libudf/src testNewChem.cpp

test.exe: newChem.o testNewChem.o
    g++ -g testNewChem.o newChem.o $(CANTERA_LIB) -o test.exe

clean:
    rm -f *.so
    rm -f *.o
    rm -f *_wrap.cxx
```



## Modify libudf/Makefile

- One change
  - Add `.cpp` extension to list of files copied
  - This makes file recursively copy the files in `libudf/src` to the appropriate library directory
    - `libudf/lnx86/2ddp`
    - `libudf/lnx86/3d`
    - `libudf/lnx86/2ddp_host (?)`



## Modify `libudf/src/makefile`

- Add functionality of the `test makefile` to the `udf makefile`
- Define a few environment variables
  1. `$(CANTERA_DIR) = <install location>`
  2. `$(CXX_SRC) = newChem.cpp`
  3. `$(CXX_INC) = $(CANTERA_DIR)/include/cantera`
  4. `$(CXX_LIB) = $(CANTERA_DIR)/lib/cantera/1.5.4`
- Create Rule for compiling `.cpp` code
- Add `$(CXX_LIB)` to the link step



# Functions which access FLUENT's function library

Set to one if `init_newChem` has been executed

```
int is_init = 0;
```

Local variables to hold the Gas State

```
real *y;  
real T = 300;  
real p_gauge = 0.0;
```

Get/Set T,p and Y to/from FLUENT

```
void getFluentComposition(cell_t cell, Thread *thread)  
void getFluentComposition(cell_t cell, Thread *thread)
```

Initialize interface with Cantera calls: `newChem_newChem( )`

```
void init_newChem( )
```

Execute equilibrate function on a single cell

```
void equil_HP(cell_t cell, Thread *thread)
```



# Create “Hooks” into FLUENT’s execution loop

## FLUENT “hook” for initialize function

```
DEFINE_ON_DEMAND(demand_initialize)
{
    init_newChem();
}
```

## FLUENT “hook” for equilibrium function

```
DEFINE_ON_DEMAND(demand_equilirbium)
{
    if (is_init == 0) init_newChem();
    thread_loop_c( thread, domain ) {
        begin_c_loop( cell, thread ) {
            if ( FLUID_THREAD_P(thread) )
                equil_HP(cell,thread);
        }
    }
}
```



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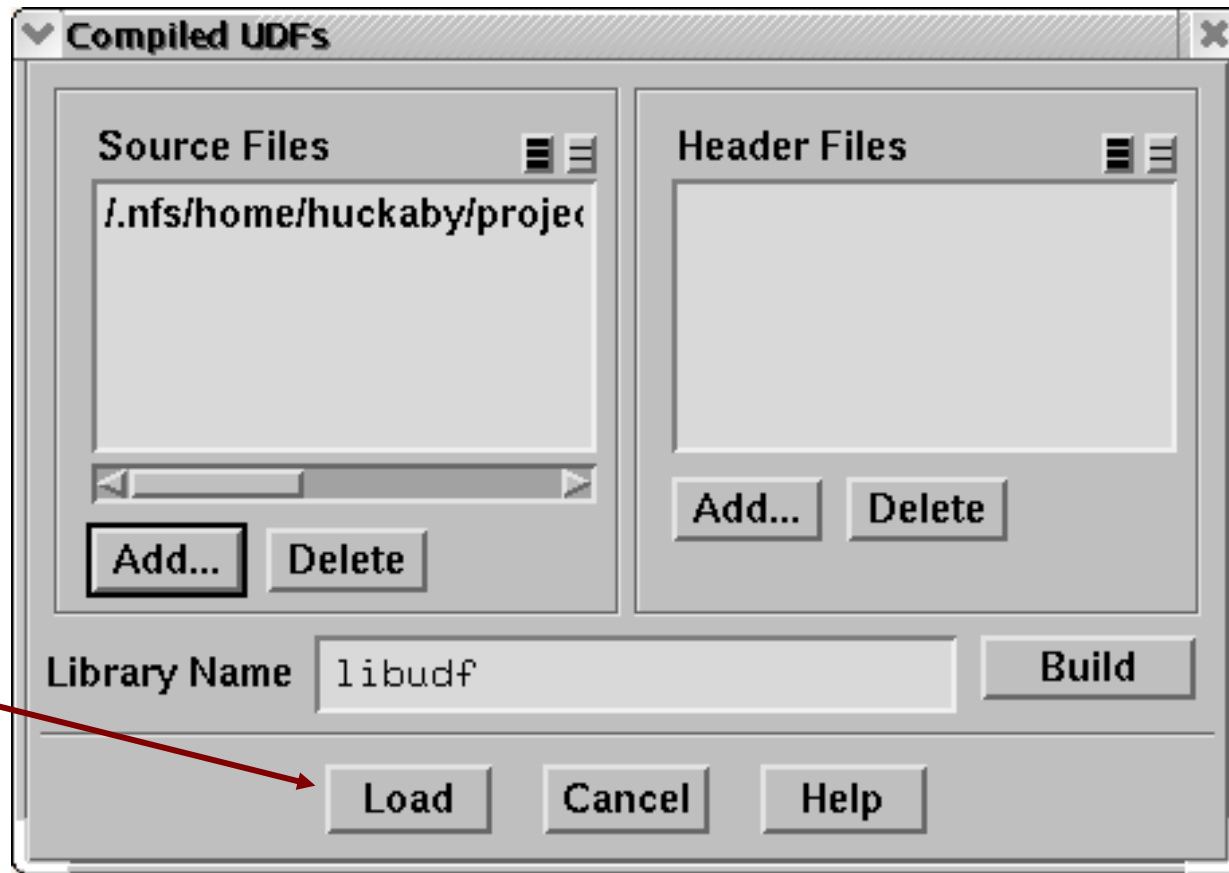
## Compile the library

- Source must be compiled **manually** as opposed to the **build** button
- Type “make” in the directory libudf



# Load the udf\_newChem into FLUENT

Define/user-defined/compiled – hit load button



# Execute demand\_initialize

The screenshot shows the FLUENT software interface. The main window displays the command window output, which includes the following text:

```
nCantera species = 53
nFluent species = 5
completed initialization of newChem.cpp
adding species 0 CH4 at position 13 to the species map
  building inverse map
adding species 1 O2 at position 3 to the species map
  building inverse map
adding species 2 CO2 at position 15 to the species map
  building inverse map
adding species 3 H2O at position 5 to the species map
  building inverse map
adding species 4 N2 at position 47 to the species map
  building inverse map
mass fraction work
end initialization of udf_
begin initialization of ud
```

An "Execute On Demand" dialog box is overlaid on the command window. The dialog box has a title bar "Execute On Demand" and a close button. It contains a "Function" dropdown menu set to "demand\_initialize", and three buttons: "Execute", "Close", and "Help". A red arrow points from the "Execute" button to the text "execute" below the dialog box. Another red arrow points from the text "Map is being built between FLUENT species and GRI 3.0 species" to the command window output.

execute

Map is being built  
between FLUENT species  
and GRI 3.0 species





# Execute demand\_equil

FLUENT@dell02.scilan [2d, dp, segregated, spe5, lam]

File	Grid	Define	Solve	Adapt	Surface	Display	Plot	Report	Parallel	Help
cell = 1060	of thread = 2	pos = -1.18663e-02, 1.57722e-03								
	3.00000e+02	-9.25253e-04	6.61018e-02	2.07771e-07	0.00000e+00	0.00000e+00	9.33898e-01			
	3.00000e+02	-9.25253e-04	6.61018e-02	2.07771e-07	0.00000e+00	0.00000e+00	9.33898e-01			
cell = 1080	of thread = 2	pos = -1.18663e-02, 2.60542e-03								
	3.00000e+02	-9.16455e-04	6.61019e-02	5.23470e-08	0.00000e+00	0.00000e+00	9.33898e-01			
	3.00000e+02	-9.16455e-04	6.61019e-02	5.23470e-08	0.00000e+00	0.00000e+00	9.33898e-01			
cell = 1100	of thread = 2	pos = -1.18663e-02, 3.73901e-03								
	3.00000e+02	-9.03940e-04	6.61019e-02	9.04384e-09	0.00000e+00	0.00000e+00	9.33898e-01			
	3.00000e+02	-9.03940e-04	6.61019e-02	9.04384e-09	0.00000e+00	0.00000e+00	9.33898e-01			
cell = 1120	of thread = 2	pos = -1.18663e-02, 7.9e-03								
	3.00000e+02	-8	6.61019e-02	1.18024e-09	0.00000e+00	0.00000e+00	9.33898e-01			
	3.00000e+02	-8	6.61019e-02	1.18024e-09	0.00000e+00	0.00000e+00	9.33898e-01			
cell = 1140	of thread = 2	pos = -1.18663e-02, 6.8e-03								
	3.00000e+02	-8	6.61019e-02	1.24258e-10	0.00000e+00	0.00000e+00	9.33898e-01			
	3.00000e+02	-8	6.61019e-02	1.24258e-10	0.00000e+00	0.00000e+00	9.33898e-01			
cell = 1160	of thread = 2	pos = -1.18663e-02, 7.9e-03								
	3.00000e+02	-9.09719e-04	6.61019e-02	6.50662e-12	0.00000e+00	0.00000e+00	9.33898e-01			
	3.00000e+02	-9.09719e-04	6.61019e-02	6.50662e-12	0.00000e+00	0.00000e+00	9.33898e-01			
cell = 1180	of thread = 2	pos = -1.18663e-02, 9.56062e-03								
	3.00000e+02	-9.18501e-04	6.61019e-02	0.00000e+00	0.00000e+00	0.00000e+00	9.33898e-01			
	3.00000e+02	-9.18501e-04	6.61019e-02	0.00000e+00	0.00000e+00	0.00000e+00	9.33898e-01			
cell = 1200	of thread = 2	pos = -1.18663e-02, -8.70278e-03								
	3.00000e+02	-8.14303e-04	0.00000e+00	2.43670e-01	0.00000e+00	0.00000e+00	7.56330e-01			
	3.00000e+02	-8.14303e-04	0.00000e+00	2.43670e-01	0.00000e+00	0.00000e+00	7.56330e-01			
cell = 1220	of thread = 2	pos = -1.18663e-02, -7.10771e-03								
	3.00000e+02	-8.00330e-04	0.00000e+00	2.43670e-01	0.00000e+00	0.00000e+00	7.56330e-01			
	3.00000e+02	-8.00330e-04	0.00000e+00	2.43670e-01	0.00000e+00	0.00000e+00	7.56330e-01			
cell = 1240	of thread = 2	pos = -1.18663e-02, -5.66093e-03								
	3.00000e+02	-7.87792e-04	7.34294e-11	2.43670e-01	0.00000e+00	0.00000e+00	7.56330e-01			
	3.00000e+02	-7.87792e-04	7.34294e-11	2.43670e-01	0.00000e+00	0.00000e+00	7.56330e-01			
cell = 1260	of thread = 2	pos = -1.18663e-02, -4.34866e-03								
	3.00000e+02	-7.86799e-04	8.33486e-10	2.43670e-01	0.00000e+00	0.00000e+00	7.56330e-01			
	3.00000e+02	-7.86799e-04	8.33486e-10	2.43670e-01	0.00000e+00	0.00000e+00	7.56330e-01			
cell = 1280	of thread = 2	pos = -1.18663e-02, -3.15839e-03								
	3.00000e+02	-7.96594e-04	5.64344e-09	2.43670e-01	0.00000e+00	0.00000e+00	7.56330e-01			
	3.00000e+02	-7.96594e-04	5.64344e-09	2.43670e-01	0.00000e+00	0.00000e+00	7.56330e-01			

Execute On Demand

Function demand\_equilt

Execute Close Help



# Confined Reacting Mixing Layer

- **Geometry:**

- Injectors:  $H = 1 \text{ cm}$ ,  $L = 4 \text{ cm}$
- Chamber:  $H = 2 \text{ cm}$ ,  $L = 20 \text{ cm}$

- **Chemistry:** 1 step – methane-air oxidation

- **Boundary Conditions:**

- \*Air inlet:  $V = 16 \text{ cm/s}$ ,  $Y_{\text{O}_2} = 0.24367$ ,  $T = 300\text{K}$
- \*Fuel inlet:  $V = 16 \text{ cm/s}$ ,  $Y_{\text{CH}_4} = 0.0661$ ,  $T = 300\text{K}$
- Walls: adiabatic, non-reacting
- Outlet: constant pressure,  $p = 1 \text{ atm}$

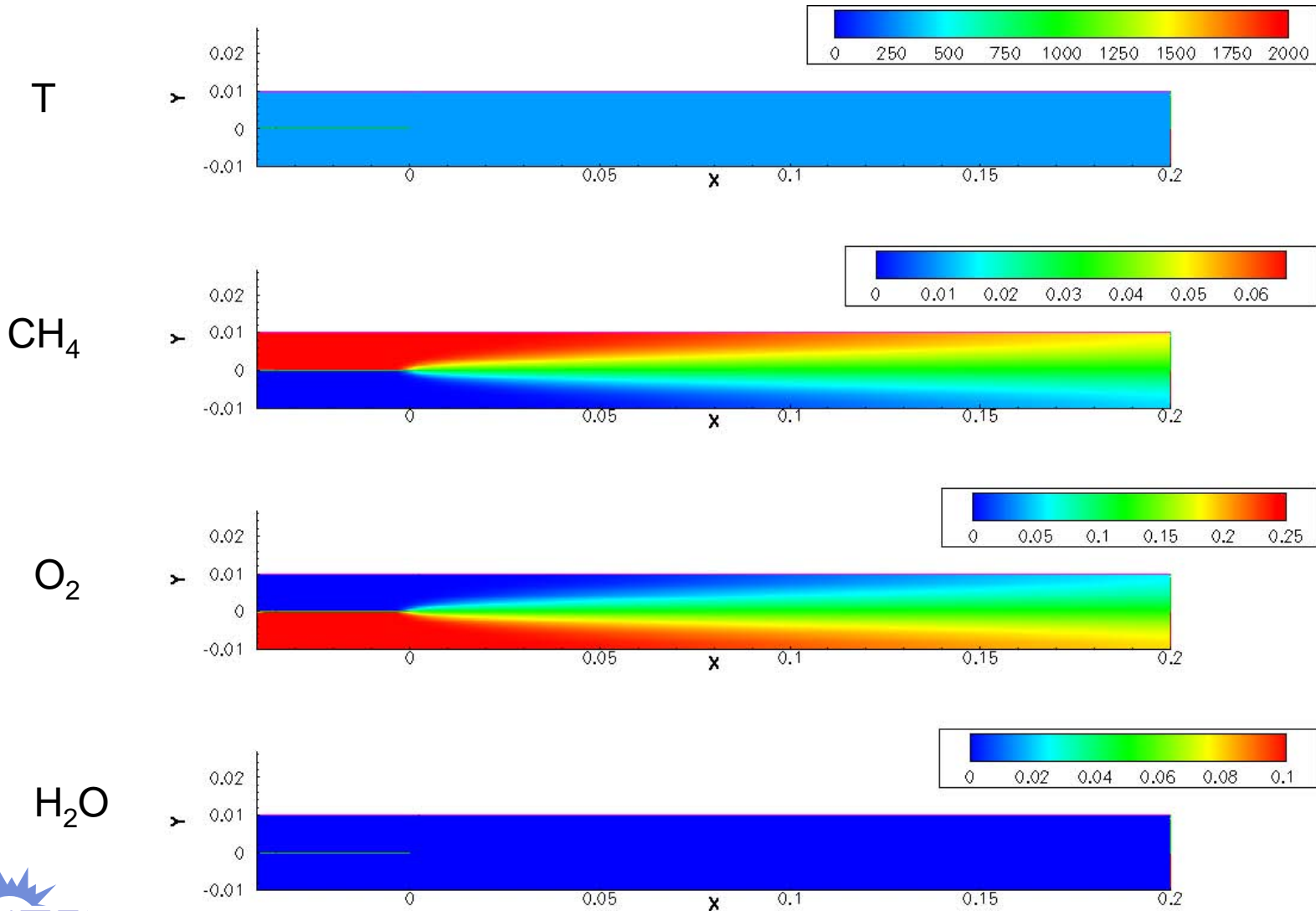
- **Solver:**

- velocity-pressure coupling - SIMPLE
- $u$ ,  $v$ ,  $T$ ,  $\rho$ ,  $Y$  - QUICK
- $p$  - 2<sup>nd</sup>-order

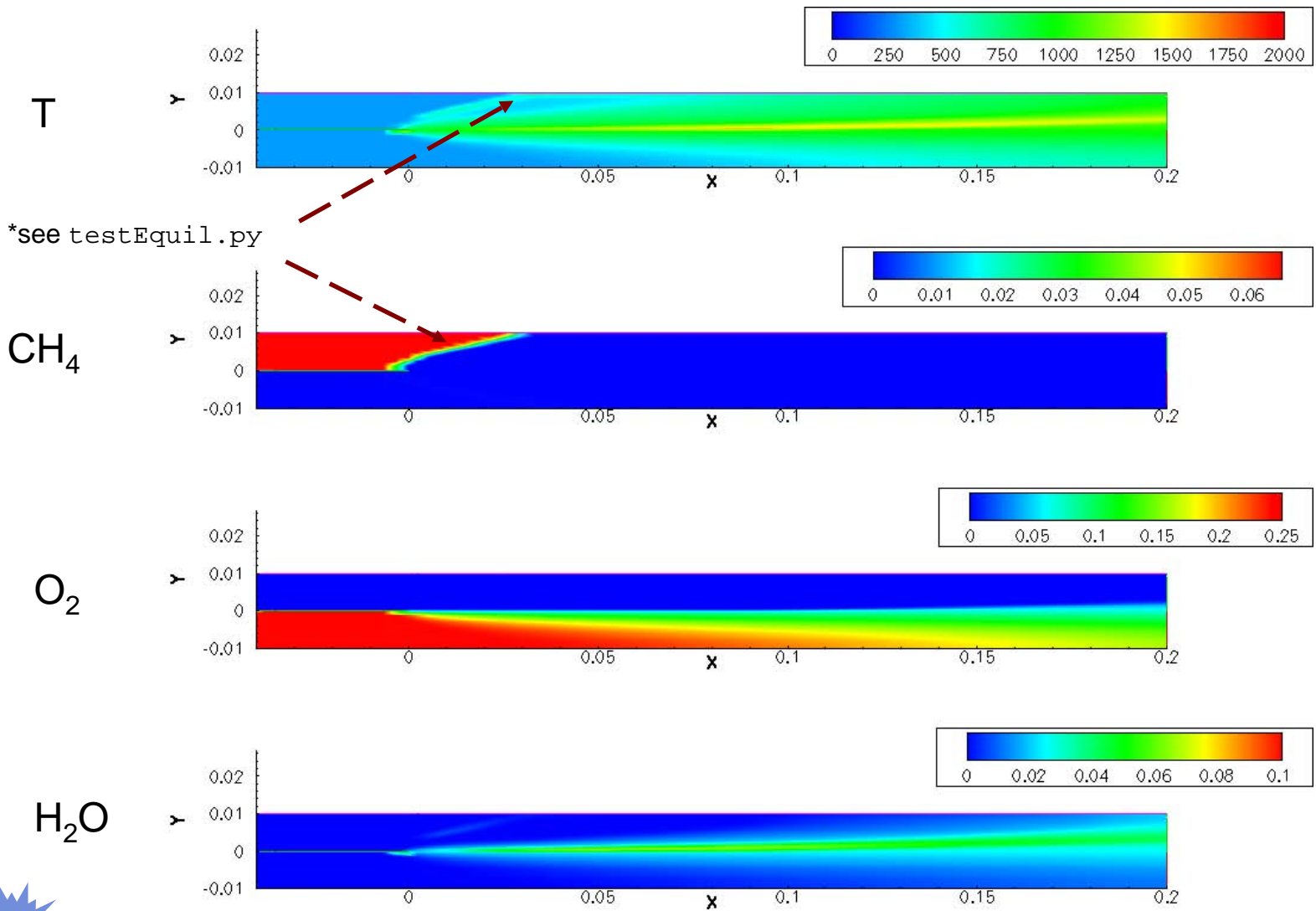
\* Jones and Becker (Comb. Flame 19, 351)



# Before demand\_equil



# After demand\_equil



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## Contact Information

- Please contact me if you have any questions or find errors in the text or example files
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