# DeepFlame

*Release 0.1*

**DeepModeling**

**Apr 14, 2023**

# QUICK START

DeepFlame is a deep learning empowered computational fluid dynamics package for single or multiphase, laminar or turbulent, reacting flows at all speeds. It aims to provide an open-source platform to combine the individual strengths of OpenFOAM, Cantera, and PyTorch libraries for deep learning assisted reacting flow simulations. It also has the scope to incorporate next-generation heterogenous supercomputing and AI acceleration infrastructures such as GPU and FPGA.

The deep learning algorithms and models used in the DeepFlame tutorial examples are developed and trained independently by our collaborator team – DeepCombustion. Please refer to their website for detailed information.

**Note:** This project is under active development.

CHAPTER

ONE

# INSTALLATION

## 1.1 Prerequisites

The installation of DeepFlame is simple and requires **OpenFOAM-7**, **LibCantera**, and **PyTorch**.

**Note:** If Ubuntu is used as the subsystem, please use Ubuntu:20.04 instead of the latest version. OpenFOAM-7 accompanied by ParaView 5.6.0 is not available for Ubuntu-latest.

First install OpenFOAM-7 if it is not already installed.

```
sudo sh -c "wget -O - https://dl.openfoam.org/gpg.key | apt-key add -"
sudo add-apt-repository http://dl.openfoam.org/ubuntu
sudo apt-get update
sudo apt-get -y install openfoam7
```

OpenFOAM-7 and ParaView-5.6.0 will be installed in the `/opt` directory.

**Note:** There is a commonly seen issue when installing OpenFOAM via `apt-get install` with an error message: `could not find a distribution template for Ubuntu/focal`. To resolve this issue, you can refer to issue#54.

**LibCantera** and **PyTorch** can be easily installed via conda. If you have compatible platform, run the following command to install DeepFlame.

```
conda create -n deepflame python=3.8
conda activate deepflame
conda install -c cantera libcantera-devel
conda install pytorch torchvision torchaudio pytorch-cuda=11.6 -c pytorch -c nvidia
conda install pybind11
conda install -c conda-forge easydict
```

**Note:** Please go to PyTorch's official website to check your system compatability and choose the installation command line that is suitable for your platform.

**Note:** Check your `Miniconda3/envs/deepflame` directory and make sure the install was successful (lib/ include/ etc. exist).

## 1.2 Configure

**1. Source your OpenFOAM-7 bashrc to configure the $FOAM environment.**

**Note:** This depends on your own path for OpenFOAM-7 bashrc.

If you have installed using `apt-get install`, then:

```
source /opt/openfoam7/etc/bashrc
```

If you compiled from source following the official guide, then:

```
source $HOME/OpenFOAM/OpenFOAM-7/etc/bashrc
```

**Note:** Check your environment using `echo $FOAM_ETC` and you should get the directory path for your OpenFOAM-7 bashrc you just used in the above step.

**2. Clone the DeepFlame repository:**

```
git clone https://github.com/deepmodeling/deepflame-dev.git
```

**3. Configure the DeepFlame environment:**

```
cd deepflame-dev
. configure.sh --use_pytorch
source ./bashrc
```

**Note:** Check your environment using `echo $DF_ROOT` and you should get the path for the `deepflame-dev` directory.

## 1.3 Build and Install

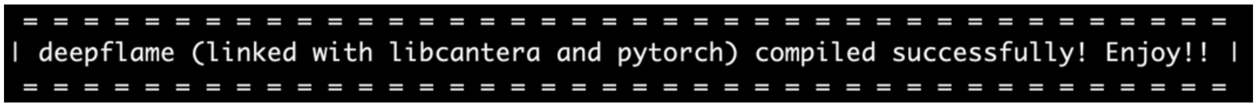
Finally you can build and install DeepFlame:

```
. install.sh
```

**Note:** You may come accross an error regarding shared library `libmkl_rt.so.2` when libcantera is installed through cantera channel. If so, go to your conda environment and check the existance of `libmkl_rt.so.2` and `libmkl_rt.so.1`, and then link `libmkl_rt.so.2` to `libmkl_rt.so.1`.

```
cd ~/miniconda3/envs/deepflame/lib
ln -s libmkl_rt.so.1 libmkl_rt.so.2
```

**If you have compiled DeepFlame successfully, you should see the print message in your terminal:**



```
= = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = 
| deepflame (linked with libcantera and pytorch) compiled successfully! Enjoy!! |
= = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = 
```

## 1.4 Other Options

DeepFlame also provides users with LibTorch and CVODE (no DNN version) options.

**1. If you choose to use LibTorch (C++ API for Torch), first create the conda env and install** LibCantera:

```
conda create -n df-libtorch
conda activate df-libtorch
conda install -c cantera libcantera-devel
```

Then you can pass your own libtorch path to DeepFlame.

```
cd deepflame-dev
. configure.sh --libtorch_dir /path/to/libtorch/
source ./bashrc
. install.sh
```

**Note:** Some compiling issues may happen due to system compatability. Instead of using conda installed Cantera C++ lib and the downloaded Torch C++ lib, try to compile your own Cantera and Torch C++ libraries.

**2. If you just need DeepFlame's CVODE solver without DNN model, just install LibCantera via** conda.

```
conda create -n df-notorch
conda activate df-notorch
conda install -c cantera libcantera-devel
```

If the conda env `df-notorch` is activated, install DeepFlame by running:

```
cd deepflame-dev
. configure.sh
source ./bashrc
. install.sh
```

If `df-notorch` not activated (or you have a self-complied libcantera), specify the path to your libcantera:

```
. configure.sh --libcantera_dir /your/path/to/libcantera/
source ./bashrc
. install.sh
```

**3. If you wish to employ the AMGX library for accelerating PDE solving using GPU:**

To begin, you will need to install AMGX. You can find the instructions for installing AMGX on its official website. Follow the instructions provided to install AMGX on your system. Once you have installed AMGX, navigate to the DeepFlame directory and follow the commands below.

```
cd ${DF_ROOT}/src/dfMatrix/solver/amgx/
export AMGX_DIR=/your/path/to/AMGX/
cmake -B build
```

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```
cd build
make
```

After this, two libraries for enabling DeepFlame with AMGX are available in `${DF_ROOT}/src/dfMatrix/solver/amgx/build`. Beforing using AMGX, run:

```
export LD_LIBRARY_PATH=${DF_ROOT}/src/dfMatrix/solver/amgx/build:$LD_LIBRARY_PATH
```

If you want to use AMGX, you will need to add configuration files for AMGX for each euqation under `system` folder and name them in the pattern of `amgxpOptions`, `amgxUOptions` . Please refer to the AMGX official website to find out detailed instructions.

**4. If you wish to install DeepFlame with CMake**

**Note:** This is still under developement.

You will need to follow the same procedures to install prerequisites and configure DeepFlame.

```
cd deepflame-dev
. configure.sh --use_pytorch
source ./bashrc
```

After this, first install libraries:

```
cd $DF_ROOT
cmake -B build
cd build
make install
```

Now if go to `$DF_ROOT/lib`, libraries should be ready. Compilition of solvers are separated. Choose the solver you want to use and then go to the directory and build it. For example,

```
cd $DF_ROOT/applications/solvers/dfLowMachFoam
cmake -B build
cd build
make install
```

CHAPTER

TWO

# DOWNLOAD DNN MODELS

The neural network models used in the tutorial examples are indepentently trained by our collaborators team – Deep-Combustion. To run DeepFlame with DNN, first download the DeepCombustion repository into `deepflame-dev/`:

```
cd $DF_ROOT
git clone https://github.com/deepcombustion/deepcombustion.git
```

Then copy the required DNN model into `mechanisms/`, for example:

```
cp -r deepcombustion/DeePCK/Model/HE04_Hydrogen_ESH2_GMS_sub_20221101/ mechanisms/
```

**Note:** Here `HE04_Hydrogen_ESH2_GMS_sub_20221101` is the default DNN model for all the tutorial cases in `$DF_ROOT/examples/`.

CHAPTER

# THREE

# TWO EXAMPLES

## 3.1 DeepFlame with DNN

If you choose to use PyTorch as the integratgor and use the compilation flag *–use_pytorch*, you can run examples stored in *$HOME/deepflame-dev/examples/.../pytorchIntegratgor*. To run an example, you first need to source your OpenFOAM:

```
source $HOME/OpenFOAM/OpenFOAM-7/etc/bashrc
```

Then, source your DeepFlame:

```
source $HOME/deepflame-dev/bashrc
```

Next, you can go to the directory of any example case that you want to run. For example:

```
cd $HOME/deepflame-dev/examples/df0DFoam/zeroD_cubicReactor/H2/pytorchIntegratgor
```

This is an example for the zero-dimensional hydrogen combustion with PyTorch as the integrator. Networks used are stored in the *mechanisms* folder, and the inference file is *inference.py*. Configurations regarding DNN are included in *constant/CanteraTorchProperties*.

The case is run by simply typing:

```
./Allrun
```

**Note:** Users can go to *constant/CanteraTorchProperties* and check if *torch* is switched on. Switch it *on* to run DNN cases, and switch *off* to run CVODE cases.

If you plot PyTorch's result together with CVODE's result, the graph is expected to look like:

## 3.2 DeepFlame without DNN

CVODE Integrator is the one without the application of Deep Neural Network (DNN). Follow the steps below to run an example of CVODE. Examples are stored in the directory: .. code-block:: bash

$HOME/deepflame-dev/examples

To run these examples, first source your OpenFOAM, depending on your OpenFOAM path:

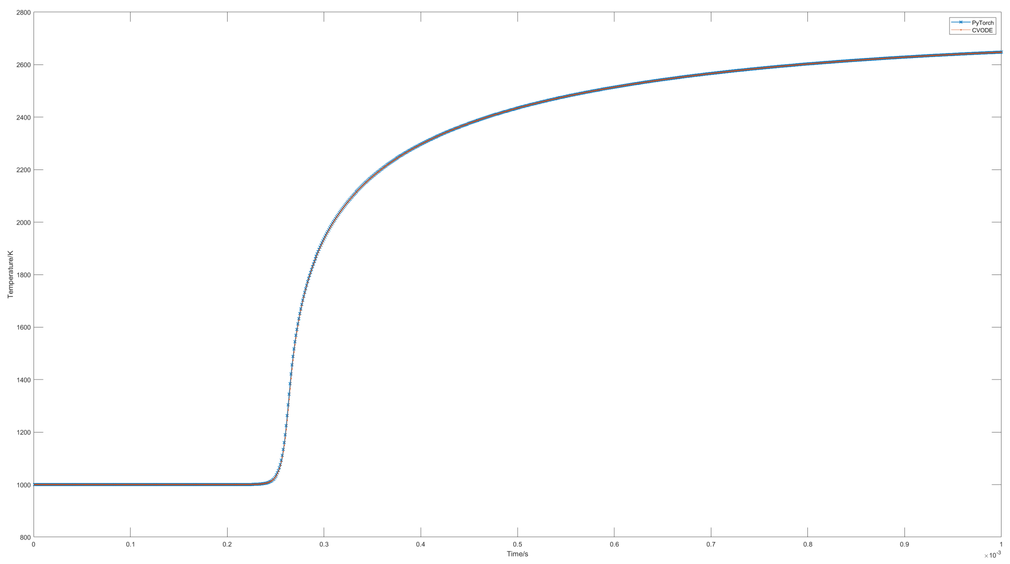

Fig. 1: Visualisation of 0D results from PyTorch and CVODE integrators

```
source $HOME/OpenFOAM/OpenFOAM-7/etc/bashrc
```

Then, source your DeepFlame:

```
source $HOME/deepflame-dev/bashrc
```

Next, you can go to the directory of any example case that you want to run. For example:

```
cd $HOME/deepflame-dev/examples/df0DFoam/zeroD_cubicReactor/H2/cvodeIntegrator
```

This is an example for the zero-dimensional hydrogen combustion with CVODE integrator.

The case is run by simply typing:

```
./Allrun
```

The probe used for post processing is defined in `/system/probes`. In this case, the probe is located at the coordinates (0.0025 0.0025 0.0025) to measure temperature variation with time. If the case is successfully run, the result can be found in `/postProcessing/probes/0/T`, and it can be visualized by running:

```
gnuplot
plot "/your/path/to/postProcessing/probes/0/T"
```

You will get a graph:

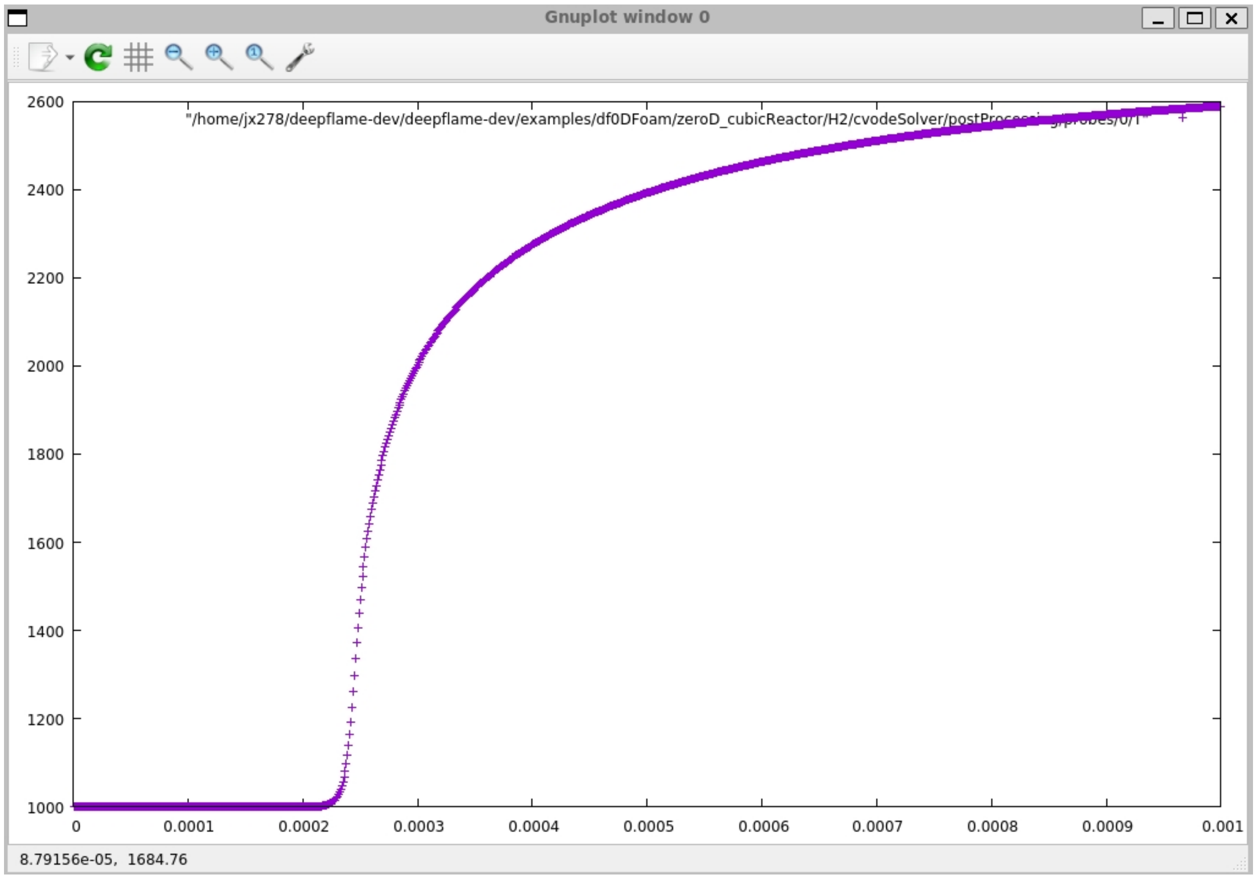

Fig. 2: Visualisation of the zero-dimensional hydrogen combustion result with CVODE integrator

CHAPTER

FOUR

# BRIEF INTRODUCTION TO INPUTS

The dictionary `CanteraTorchProperties` is the original dictionary of DeepFlame. It reads in network related parameters and configurations. It typically looks like:

```
chemistry           on;
CanteraMechanismFile "ES80_H2-7-16.yaml";
transportModel "Mix";
odeCoeffs
{
    "relTol"   1e-15;
    "absTol"   1e-24;
}
inertSpecie        "N2";
zeroDReactor
{
    constantProperty "pressure";
}

splittingStretagy false;

TorchSettings
{
    torch on;
    GPU   off;
    log   on;
    torchModel "HE04_Hydrogen_ESH2_GMS_sub_20221101";
    coresPerNode 4;

}
loadbalancing
{
        active  false;
        //log   true;
}
```

In the above example, the meanings of the parameters are:

- `CanteraMechanismFile`: the name of the reaction mechanism file.
- `transportModel`: the default model is *Mix*, but other models including *UnityLewis* and *Multi* are also availabile.
- `constantProperty`: property set to be constant during reaction. It can be set to *pressure* or *volume*.

- odeCoeffs: the ode tolerance. 1e-15 and 1e-24 are used for network training, so they should be kept the same when comparing results with and without DNN. Default values are 1e-9 and 1e-15.
- TorchSettings: all paramenters regarding the usage of DNN. This section will not be read in CVODE cases.
- torch: the switch used to control the on and off of DNN. If users are running CVODE, this needs to be switched off.
- GPU: the switch used to control whether GPU or CPU is used to carry out inference.
- torchModel: name of network.
- coresPerNode: If you are using one node on a cluster or using your own PC, set this parameter to the actual number of cores used to run the task. If you are using more than one node on a cluster, set this parameter the total number of cores on one node. The number of GPUs used is auto-detected.

The dictionary combustionProperties is the original dictionary of DeepFlame. It reads in network related parameters and configurations. It typically looks like:

```
combustionModel  flareFGM;//PaSR,EDC

EDCCoeffs
{
    version v2005;
}

PaSRCoeffs
{
   mixingScale
   {
      type   globalScale;//globalScale,kolmogorovScale,geometriMeanScale,dynamicScale
      globalScaleCoeffs
      {
        Cmix  0.01;
      }

      dynamicScaleCoeffs
      {
        ChiType      algebraic;// algebraic; transport;
      }
    }
   chemistryScale
   {
      type  globalConvertion;//formationRate,globalConvertion
      globalConvertionCoeffs
      {
           fuel CH4;
           oxidizer O2;
      }
   }

}

flareFGMCoeffs
{
  buffer           false;
```

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```
  scaledPV         false;
  combustion       false;
  ignition         false;
  solveEnthalpy    false;
  flameletT        false;
  relaxation       false;
  DpDt             false;
/*ignition         false;
  ignBeginTime     0.1;
  ignDurationTime  0.0;
  x0               0.0;
  y0               0.0;
  z0               0.0;
  R0               0.0;*/
  Sct              0.7;
  bufferTime       0.0;
  speciesName      ("CO");
}
```

In the above example, the meanings of the parameters are:

- `combustionModel`: the name of the combustion model, alternative models include PaSR, EDC, flareFGM.
- `EDCCoeffs, PaSRCoeffs, flareFGMCoeffs`: model cofficients we need to define.
- `mixingScale`: turbulent mixing time scale including globalScale,kolmogorovScale,geometriMeanScale,dynamicScale.
- `ChiType`: algebraic and transport are available for ChiType when selecting dynamicScale.
- `chemistryScale`: chemistry reaction time scale including formationRate,globalConvertion .
- `buffer`: switch for buffer time.
- `scaledPV`:the switch is used to determine whether to use scaled progress variables or not.
- `combustion`:the switch is used to control whether the chemical reactions are on or off.
- `ignition`:the switch is used to control whether the ignition is on or off.
- `solveEnthalpy`:the switch is used to determine whether to solve enthalpy equation or not.
- `flameletT`:the switch is used to determine whether to read flame temperature from table or not.
- `relaxation`:the switch is used to determine whether to use relaxation iteration for transport equations or not.
- `DpDt`:the switch is used to determine whether to include material derivatives or not.
- `ignBeginTime`:beginning time of ignition.
- `ignDurationTime`:duration time of ignition.
- `x0, y0, z0`:coordinate of ignition center.
- `R0`:radius of ignition region.
- `Sct`:turbulent Schmidt number, default value is set as 0.7.
- `speciesName`:name of species we need to lookup.

CHAPTER

FIVE

# DF0DFOAM

## 5.1 Zero-Dimensional ignition reactor

**Problem Description**

This case simulates the zero-dimensional autoignition under constant-pressure or constant-volume condition. This case confirm the validity of the implementation of chemical reaction source terms in DeepFlame.

Table 1: Operating Conditions in Brief

| | |
|---|---|
| Mixture | Hydrogen-Air |
| Equivalence Ratio | 1.0 |
| Initial Gas Temperature | 1400 K |
| Initial Gas Pressure | 1 atm |

**Output**

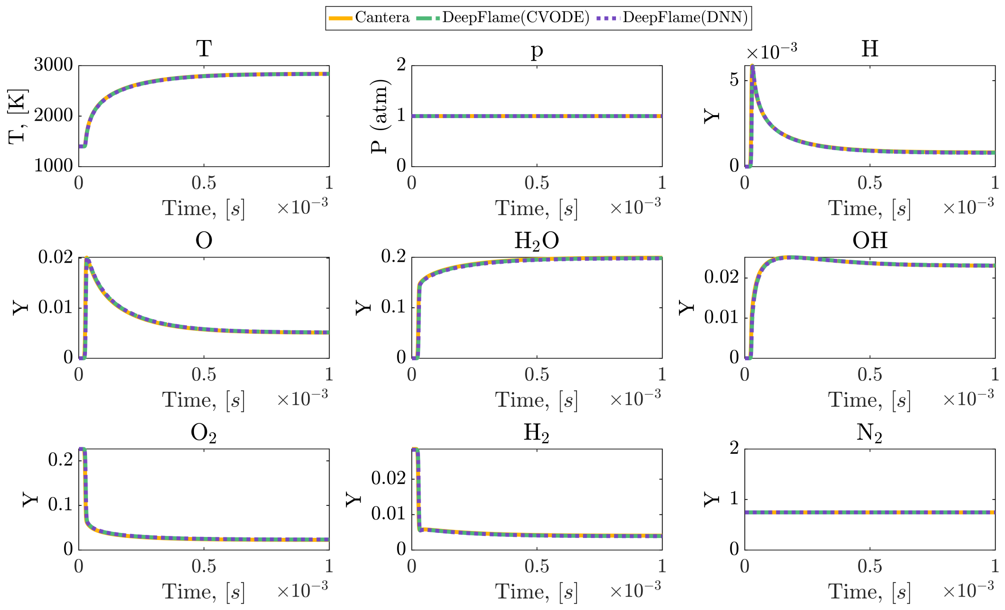


Fig. 1: Results of zero-dimensional constant-pressure autoignition

CHAPTER

SIX

# DFLOWMACHFOAM

## 6.1 One-Dimensional Planar Flame

**Problem Description**

The case simulates the steady-state 1D freely-propagating flame. The results are able to catch the flame thickness, laminar fame speed and the detailed 1D flame structure. This case demonstrate that the convection-diffusion-reaction algorithms implemented in our solver are stable and accurate.

Table 1: Operating Conditions in Brief

| | |
|---|---|
| Computational Domain length | 0.06 m |
| Mixture | Hydrogen-Air |
| Equivalence Ratio | 1.0 |
| Inlet Gas Temperature | 300 K |

**Output**

## 6.2 Two-Dimensional Triple Flame

**Problem Description**

This case simulates the evolution of a 2D non-premixed planar jet flame to validate the capability of our solver for multi-dimensional applications.

Table 2: Operating Conditions in Brief

| | |
|---|---|
| Computational Domain size (x) | 0.03 m * 0.05 m |
| Jet Composition | H2/N2= 1/3 (fuel jet), Air (co-flow) |
| Initial Velocity | 5 m/s (fuel jet), 1 m/s (co-flow) |
| Initial Gas Temperature | 1400 K (ignition region), 300 K (other area) |

**Output**

The initial condition and the evolution of the jet flame are presented in this figure.

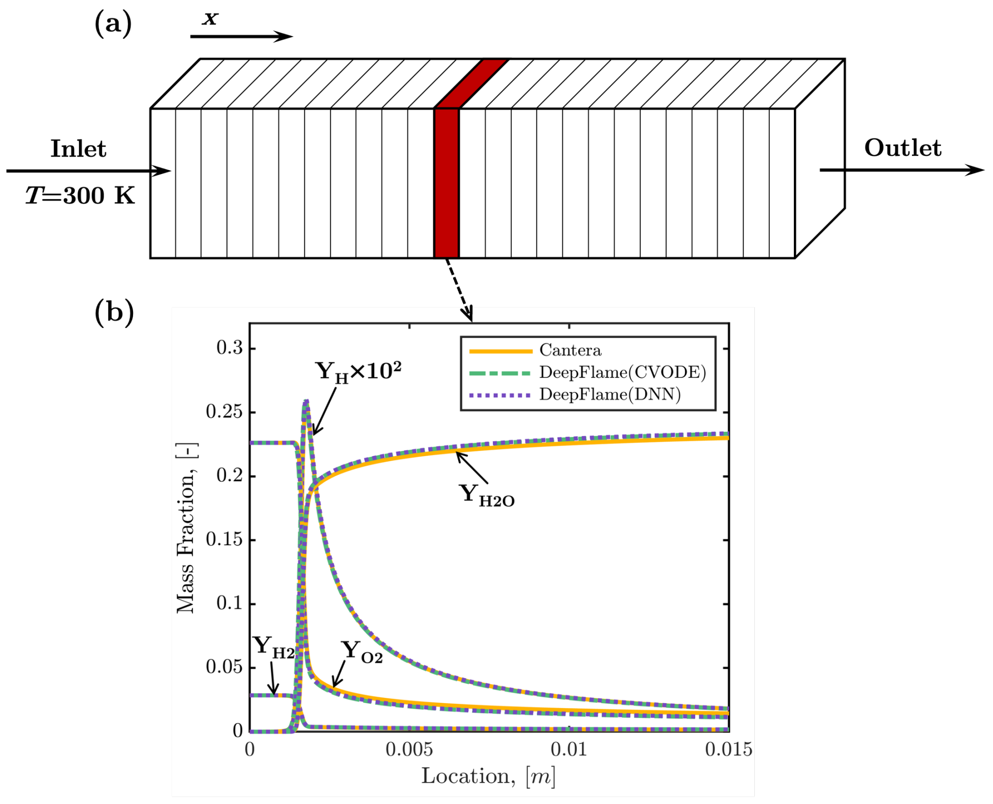


Fig. 1: Numerical setup of one-dimensional premixed flame and the detailed flame structure obtained by our solver

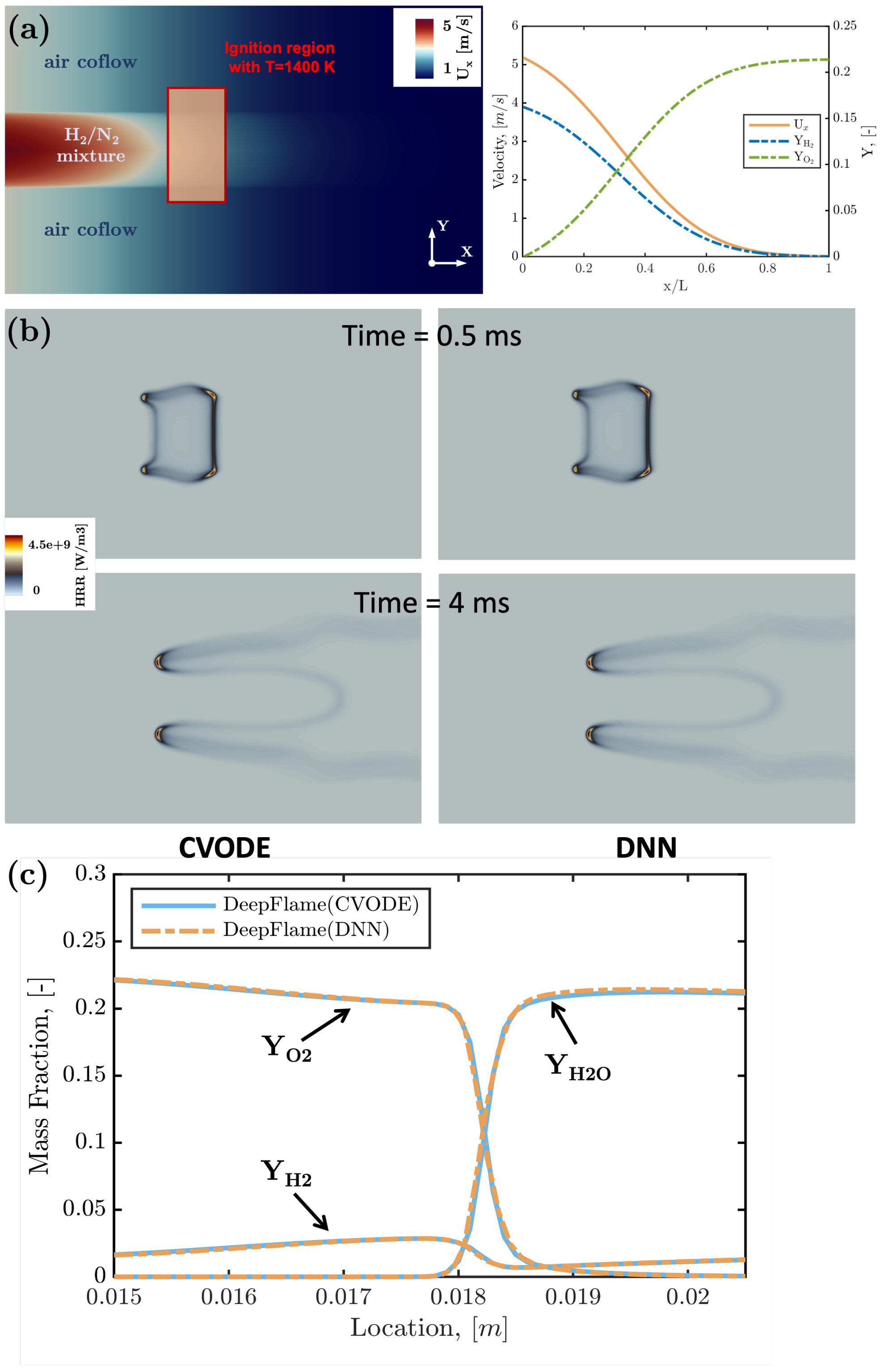


Fig. 2: Simulation results of the two-dimensional jet flame.

## 6.3 Two-Dimensional Reactive Taylor-Green Vortex

**Problem Description**

2D reactive Taylor-Green Vortex (TGV) which is simplified from the 3D reactive TGV below is simulated here. It can be used for debugging, validation of DNN models against CVODE solutions and so on.

The initial velocity, pressure and mass fraction fields are set according to a benchmark case established by Abdelsamie et al. The initial temperature of the cold gas is set to be 500 K.

**Output**

The developed 2D TGV are displayed in the figures below.

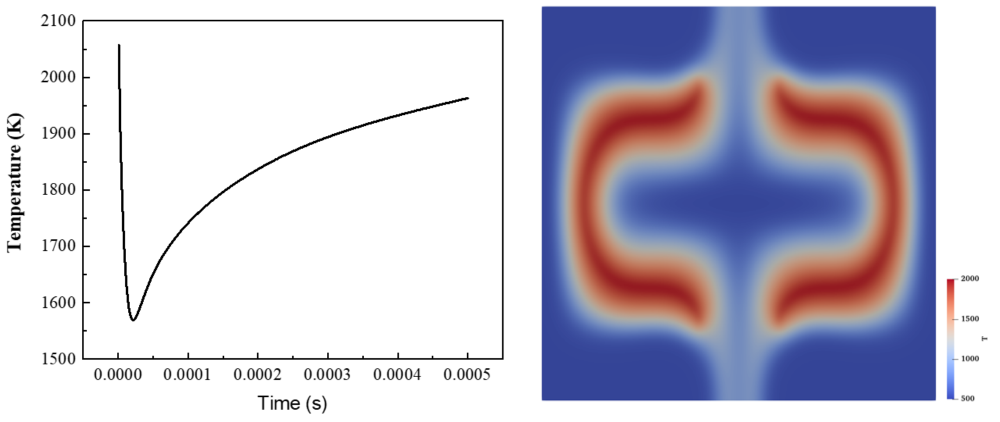


Fig. 3: Profiles of temperature history and contours of temperature and species mass fraction at t = 0.5 ms (two reference time)

**Reference**

A.Abdelsamie, G.Lartigue, C.E.Frouzakis, D.Thevenin, The taylor-green vortex as a benchmark for high-fidelity combustion simulations using low-mach solvers, Computers & Fluids 223 (2021): 104935.

## 6.4 Two-Dimensional Flame in Homogeneous Isotropic Turbulence

**Problem Description**

2D reacting flow with homogeneous isotropic turbulence (HIT) is simulated here. It can be used to simulate kinetic energy dissapation and qualitatively assess turbulence effects on combustion under the circumstances that 3D simulations are computationally prohibitive.

The domain is initially filled with CH4/air mixture with an equivalence ratio of 0.6 at atmospheric pressure. To initialize 2d HIT simulations, turbulence is generated follwing the procedure described by Vuorinen and Keskinen.

Table 3: Operating Conditions in Brief

| | |
|---|---|
| Computational Domain size (x) | 20*pi mm * 20*pi mm |
| Initial Gas Temperature | 1800 K (ignition region), 800 K (other area) |
| Ignition region | Circle in the domain center with a radius of 1/10 domain length |

The figure below shows contour of vorticity at initial time.

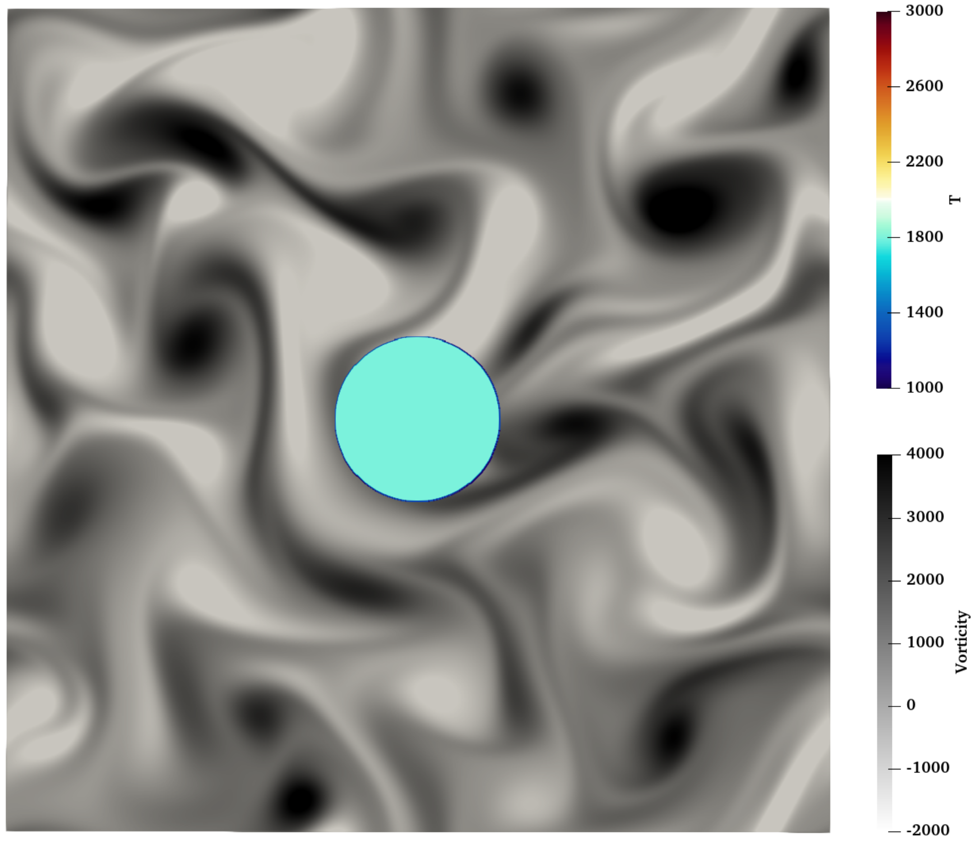


Fig. 4: Initial contours of temperature and vorticity for the 2D reactive HIT

**Output**

The developed 2D HIT are displayed in the figures below.

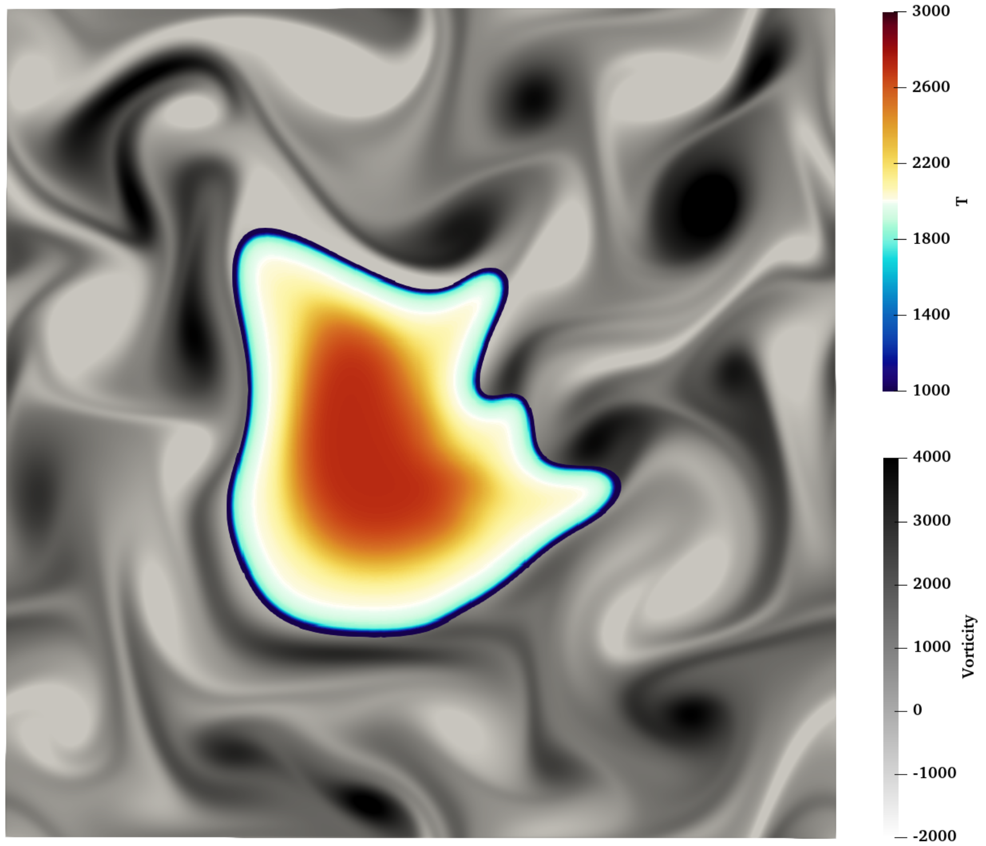


Fig. 5: Contours of temperature and vorticity at t = 1.5 ms

**Reference**

Vuorinen, Ville, and K. Keskinen. "DNSLab: A gateway to turbulent flow simulation in Matlab." Computer Physics Communications 203 (2016): 278-289.

## 6.5 Three-Dimensional Reactive Taylor-Green Vortex

3D reactive Taylor-Green Vortex (TGV) which is a newly established benchmark case for reacting flow DNS codes is simulated here to evaluate the computational performance of our solver.

The initial fields are set according to a benchmark case established by Abdelsamie et al. The figure below shows contours of vorticity magnitude and temperature as well as the x-direction profiles of species at initial time.

**Output**

The developed TGV are displayed in the figures below.

**Reference**

A.Abdelsamie, G.Lartigue, C.E.Frouzakis, D.Thevenin, The taylor-green vortex as a benchmark for high-fidelity combustion simulations using low-mach solvers, Computers & Fluids 223 (2021): 104935.

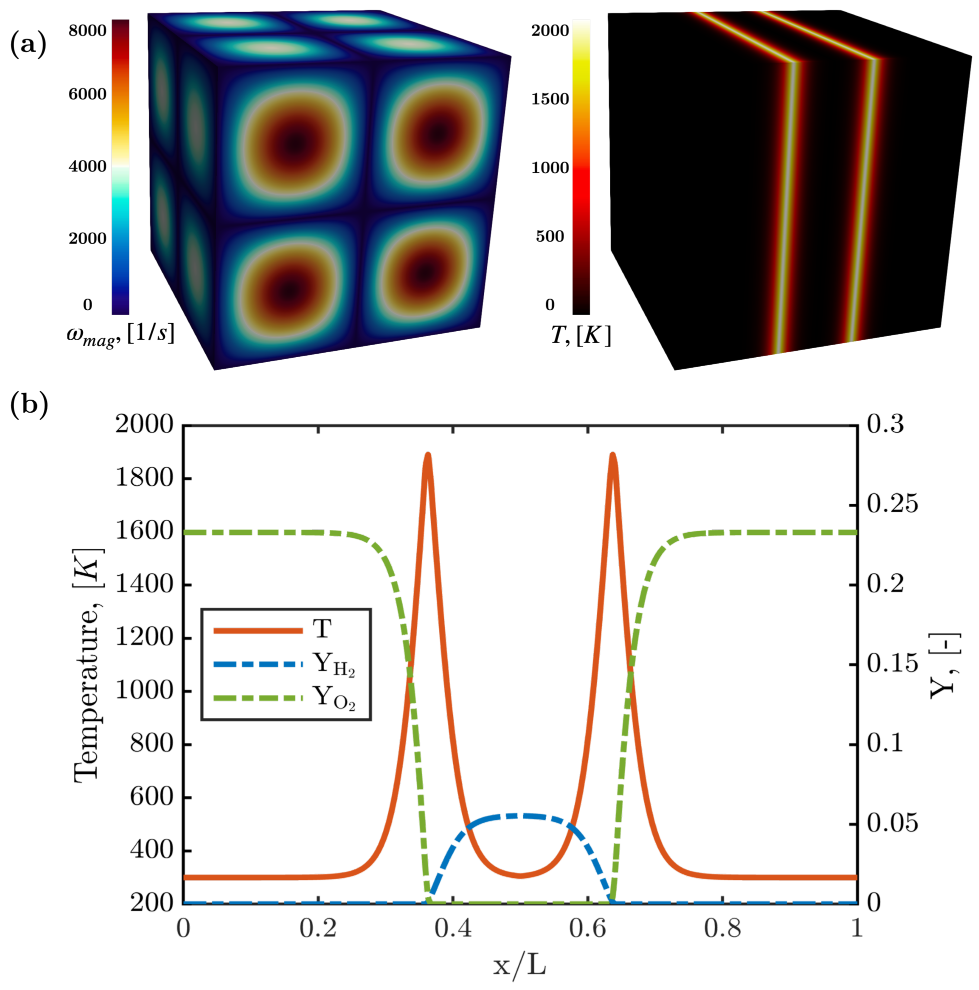


Fig. 6: Initial contours and profiles of vorticity magnitude, temperature, and species mass fraction for the reactive TGV

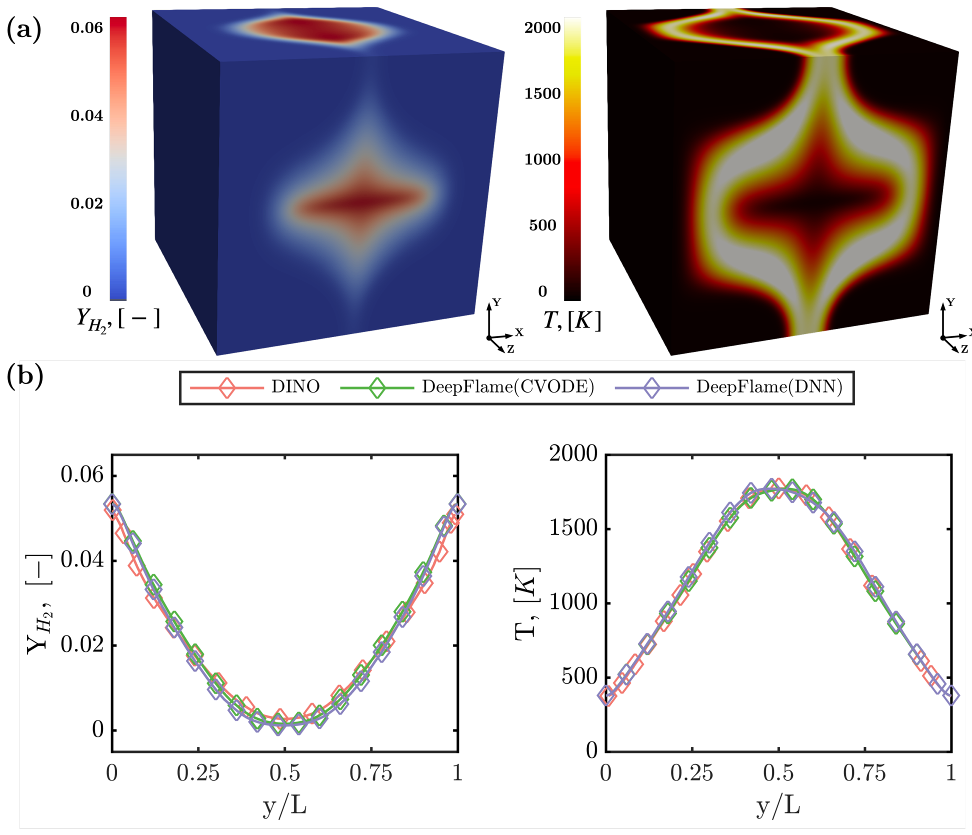


Fig. 7: Contours and profiles of temperature and species mass fraction at t = 0.5 ms

# CHAPTER SEVEN

# DFHIGHSPEEDFOAM

## 7.1 One-Dimensional Reactive Shock Tube

### Problem Description

The case simulates supersonic inlet flow hitting the wall and then reflected to ignite the premixed gas. The reactive wave will catch the reflected shock wave. This case can also verify the accuracy of our solver in capturing the interaction of convection and reaction.

Table 1: Operating Conditions in Brief

| | |
|---|---|
| Chamber size (x) | 0.12 m |
| Initial Gas Density | 0.072 kg/m^3 (x<=0.06 m), 0.18075 kg/m^3 (x>0.06 m) |
| Initial Gas Pressure | 7173 Pa (x<=0.06 m), 35594 Pa (x>0.06 m) |
| Initial Gas Velocity | 0 m/s (x<=0.06 m), -487.34 m/s (x>0.06 m) |
| Ideal Gas Composition (mole fraction) | H2/O2/Ar = 2/1/7 |

### Output

### Reference

E S Oran, T R Young, J P Boris, A Cohen, Weak and strong ignition. i. Numerical simulations of shock tube experiments, Combustion and Flame 48 (1982) 135-148.

R J Kee, J F Grcar, M D Smooke, J A Miller, E Meeks, Premix: A fortran program for modeling steady laminar one-dimensional premixed flames, Sandia National Laboratories.

## 7.2 One-Dimensional H2/Air Detonation

### Problem Description

Detonation propagation contains a complex interaction of the leading shock wave and auto-igniting reaction, showing the coupling of shock wave and chemical reaction. This case aims to validate the accuracy of this solver in capturing this process and the propagation speed.

Table 2: Operating Conditions in Brief

| | |
|---|---|
| Chamber size (x) | 0.5 m |
| Initial Gas Pressure | 90 atm (hot spot), 1 atm (other area) |
| Initial Gas Temperature | 2000 K (hot spot), 300 K (other area) |
| Ideal Gas Composition (mole fraction) | H2/O2/N2 = 2/1/3.76 (homogeneous stoichiometric mixture) |

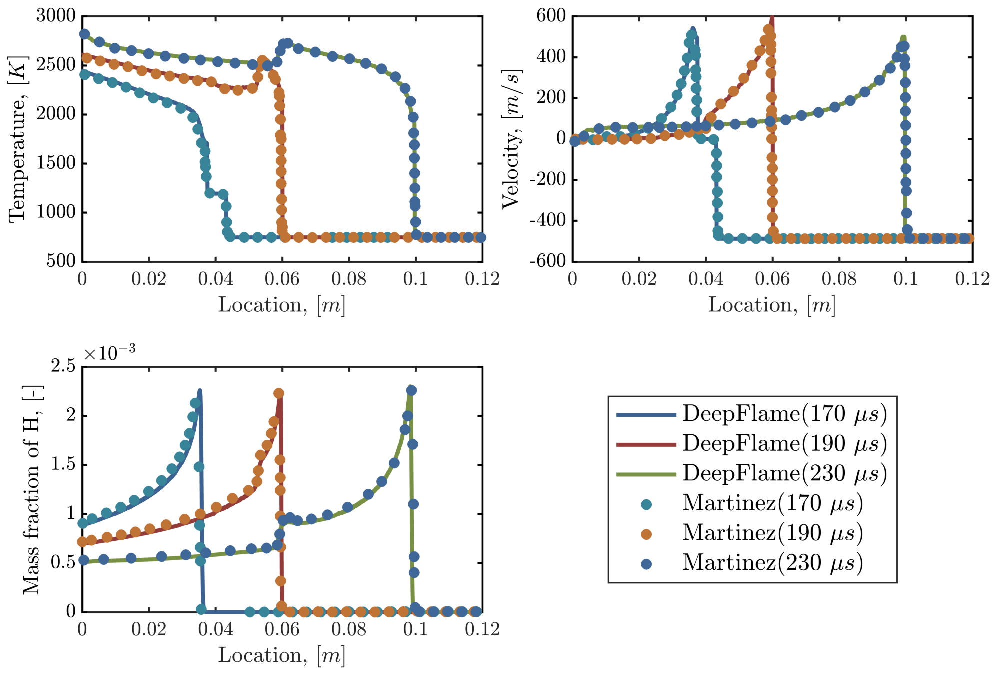


Fig. 1: Result of one-dimensional reactive shock tube

**Output**

**Reference**

J Li, Z Zhao, A Kazakov, F L Dryer, An updated comprehensive kinetic model of hydrogen combustion, International Journal of Chemical Kinetics 36 (2004) 566-575.

## 7.3 Two-Dimensional H2/Air Detonation

**Problem Description**

Detonation propagation contains a complex interaction of the leading shock wave and auto-igniting reaction, and two-dimensional detonation can further reveal the interaction of shear waves and shock waves.

Table 3: Operating Conditions in Brief

| | |
|---|---|
| Chamber size (x) | 0.2 m * 0.01 m |
| Initial Gas Pressure | 100 atm (three hot spot), 1 atm (other area) |
| Initial Gas Temperature | 2000 K (three hot spot), 300 K (other area) |
| Ideal Gas Composition (mole fraction) | H2/O2/N2 = 2/1/7 (homogeneous stoichiometric mixture) |

**Output**

Triple points can be seen clearly in the picture below.

In the picture below, during the propagation of detonation wave, we can see that the size of cells gradually became stable.

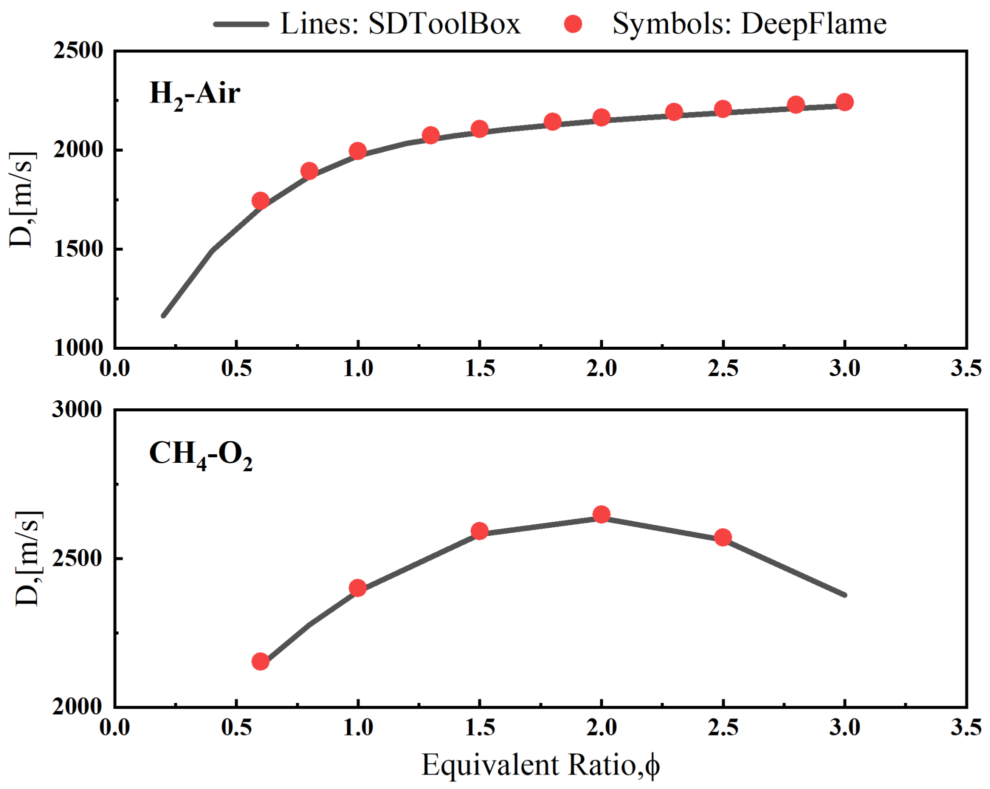


Fig. 2: Result of one-dimensional H2/air detonation

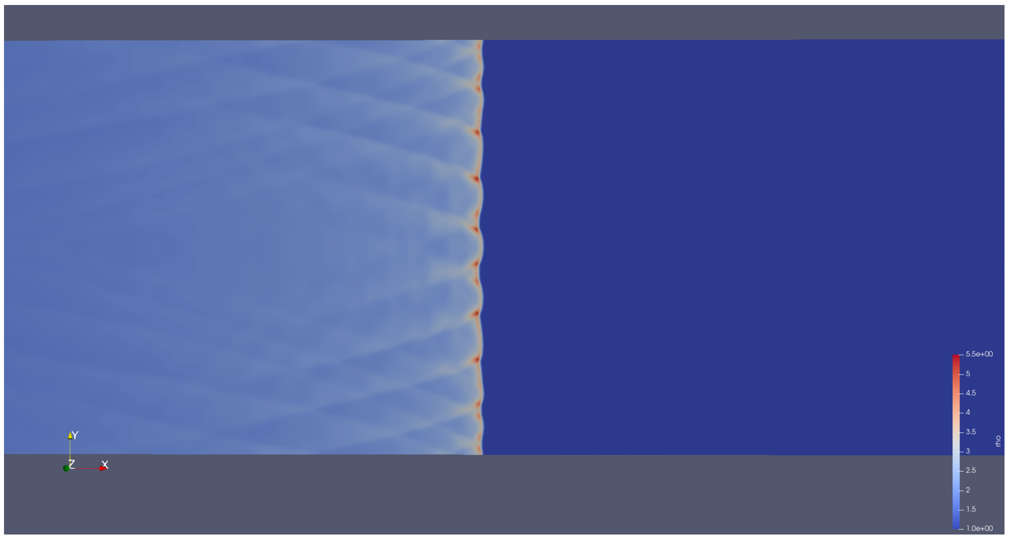


Fig. 3: Density field of two-dimensional H2 detonation

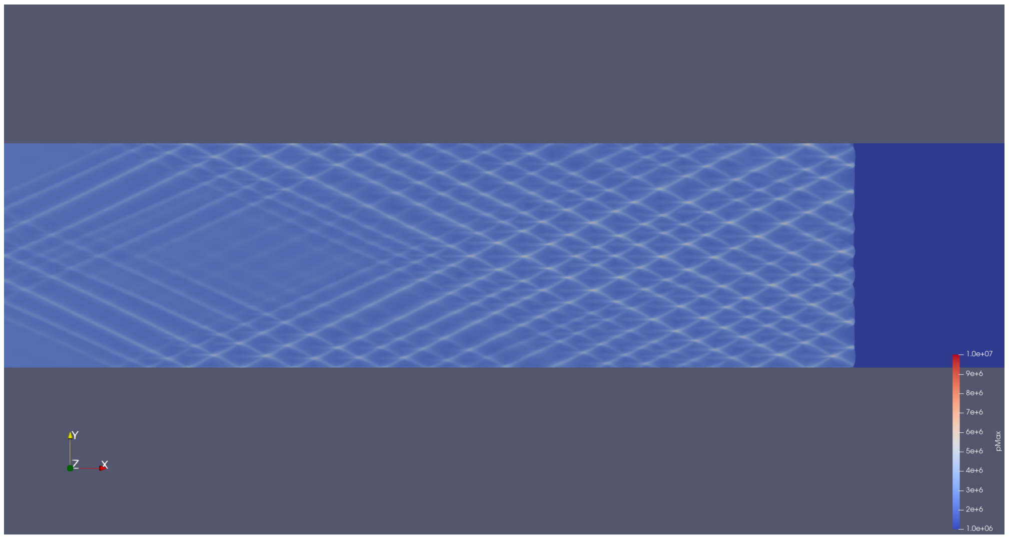


Fig. 4: History of maximum pressure during detonation propagation

**Reference**

C J Jachimowski, An Analytical Study of the Hydrogen-Air Reaction Mechanism with Application to Scramjet Combustion, NASA TP-2791, Feb. 1988.

CHAPTER

# EIGHT

# DFSPRAYFOAM

## 8.1 aachenBomb

### Problem Description

This case simulates combustion inside a constant volume chamber based on an experimental setup at RWTH Aachen University. It can mimic, for example, the beginning of power stroke in a four-stroke diesel engine.

Table 1: Operating Conditions in Brief

| | |
|---|---|
| Chamber size (xyz) | 0.02×0.1×0.02m^3 |
| Initial Gas Temperature | 800K |
| Initial Gas Pressure | 5MPa |
| Initial Gas Composition (mass fraction) | 23.4% O2, 76.6% N2 |
| Fuel | n-heptane |
| Fuel Temperature at the Nozzle | 320K |
| Fuel Injection Duration | 1.25ms |
| Total Injection Mass | 6mg |

### Configurations Different from OpenFOAM Case

Cantera is used instead of the built-in modules of OpenFOAM to solve the chemical reactions. Therefore, a chemical mechanism file in YAML format is required in the case directory, and the full name of the mechanism file ("xxx.yaml") should be the entry after the keyword **CanteraMechanismFile** in *constant/CanteraTorchProperties*. Non-reacting simulation can be conducted by switching the entry after the keyword **chemistry** from **on** to **off** in *constant/CanteraTorchProperties*.

### Results

## 8.2 Sydney Spray Burner

### Problem Description

A 2D-wedge case is used to simulate the dilute spray combustion processes inside a spray burner based on the experimental setup at Sydney University. It has been widely used for the study of droplet-chemistry-turbulence interaction.

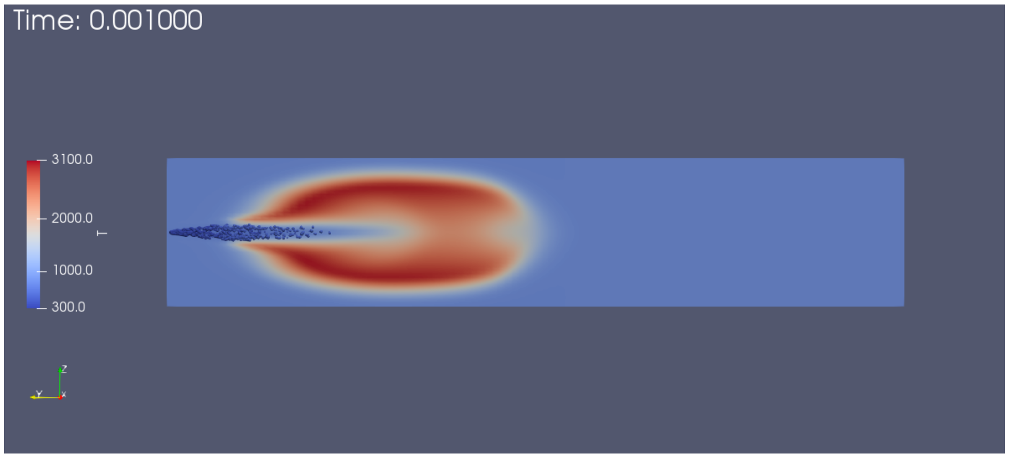


Fig. 1: Visualization of temperature contours with large particle distribution

Table 2: Operating Conditions in Brief (Details can be found for Case EtF4 in [1] )

| | |
|---|---|
| Chamber size (wedge, 4 degree) | 0.104×0.500m^2 |
| Initial Gas Temperature in Domain | 293K |
| Initial Gas Temperature at Fuel Inlet | 267K |
| Initial Gas Temperature at Pilot Inlet | 2493K |
| Initial Gas Pressure | 1Bar |
| Initial Gas Composition in Domain(mass fraction) | 23.4% O2, 76.6% N2 |
| Fuel | C2H5OH |
| Mass-flow Rate of Air Carrier | 150g/min |
| Liquid Fuel Injection Rate | 23.4g/min |
| Bulk Jet Velocity | 24m/s |
| Bulk Burned Pilot Velocity | 11.6m/s |

**Configurations Different from OpenFOAM Case**

Cantera is used instead of the built-in modules of OpenFOAM to solve the chemical reactions. Therefore, a chemical mechanism file in YAML format is required in the case directory, and the full name of the mechanism file ("xxx. yaml") should be the entry after the keyword **CanteraMechanismFile** in *constant/CanteraTorchProperties*. Non-reacting simulation can be conducted by switching the entry after the keyword **chemistry** from **on** to **off** in *constant/CanteraTorchProperties*.

**Note**

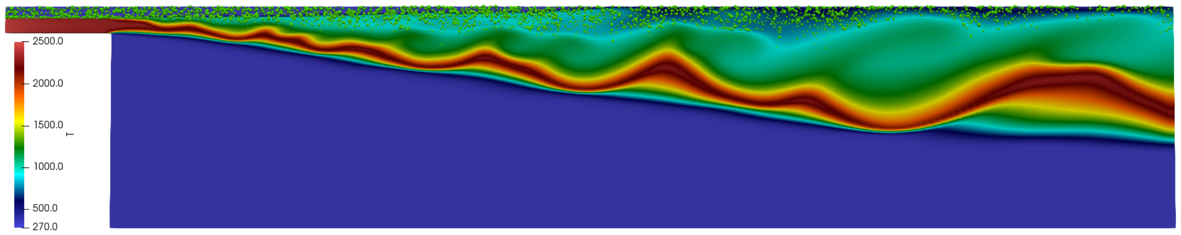
When running a wedge case with OpenFOAM, you may come across an error "**Hitting a wedge patch should not be possible**". One solution is to comment out the lines with the "**FatalErrorIn**" call in **src/lagrangian/basic/particle/particleTemplates.C**. Details can be found in the thread [2].

**Results**

**Reference**

[1] Gounder, James Dakshina, Agisilaos Kourmatzis, and Assaad Rachid Masri. "Turbulent piloted dilute spray flames: Flow fields and droplet dynamics." Combustion and flame 159.11 (2012): 3372-3397.

[2]https://www.cfd-online.com/Forums/openfoam/89003-3d-spray-vs-axisymmetric-spray-dieselfoam.html


2500.0
2000.0
1500.0
1000.0
500.0
270.0
T

CHAPTER

NINE

# REACTION MECHANISM CONVERTION

DeepFlame uses *yaml* reaction mechanisms, which are compatible with Cantera. The following command lines can be used to convert *chemkin* mechanisms into *yaml* format.

```
conda create --name ct-env --channel conda-forge cantera
conda activate ct-env
ck2yaml --input=chem.inp --thermo=therm.dat --transport=tran.dat
```

**Note:** Users will need to create a new conda environment other than the one used for DeepFlame's dependencies, and the channel needs to be `conda-forge`. Otherwise, there might be an error regarding shared library, `libmkl_rt.so.2`.

More detailed instruction of converting mechanisms can be found on Cantera official website.

# CHAPTER TEN

# FLAME SPEED

flameSpeed.C is another utility in DeepFlame. The flame is located at the maximum temperature gradient at a certain time, and its speed is equal to the maximum gradient porpagation speed subtracting the inlet speed. To use this utility, simply run the commands below after the simulation.

```
runApplication reconstructPar
flameSpeed
```

A log containing flame thickness, flame location, flame proagation speed, and flame speed at each time step will be presented.

**Note:** This utility only applies to one-dimensional cases. Similar logs can also exit when it is run for two or three dimensional cases, but results are not physical.

CHAPTER

ELEVEN

# DEVELOPERS TEAM

The current DeepFlame developers come from the following research groups/affiliations:

- Peking University (Lead PI: Zhi X. Chen)
- AI for Science Institute (AISI), Beijing

# CHAPTER TWELVE

# COLLABORATORS TEAM

- Shanghai Jiao Tong University (Lead PI: Zhi-Qin John Xu)
- Southern University of Science and Technology (Lead PI: Tianhan Zhang)

CHAPTER

THIRTEEN

# HOW TO CITE

**If you use DeepFlame for a publication, please use the citation:**

Runze Mao, Minqi Lin, Yan Zhang, Tianhan Zhang, Zhi-Qin John Xu, Zhi X. Chen. DeepFlame: A deep learning empowered open-source platform for reacting flow simulations (2022). doi:10.48550/arXiv.2210.07094

**If you have used the DNN model provided from us, please use the citation:**

Tianhan Zhang, Yuxiao Yi, Yifan Xu, Zhi X. Chen, Yaoyu Zhang, Weinan E, Zhi-Qin John Xu. A multi-scale sampling method for accurate and robust deep neural network to predict combustion chemical kinetics. Combust. Flame 245:112319 (2022). doi:10.1016/j.combustflame.2022.112319

# CHAPTER FOURTEEN

# LICENSE

The project DeepFlame is licensed under GNU General Public License v3.0

CHAPTER

FIFTEEN

# SUBMITTING A PULL REQUEST

We welcome contributions from the open source community. The main approach to communicate with and to make contribution to DeepFlame is to open a pull request.

1. Fork the DeepFlame repository.
2. Pull your forked repository, and create a new git branchmake to your changes in it:

```
git checkout -b my-fix-branch
```

3. Coding your patch
4. After tests passed, commit your changes with a proper message.
5. Push your branch to GitHub:

```
git push origin my-fix-branch
```

6. In GitHub, send a pull request with `deepmodeling/deepflame-dev` as the base repository.
7. After your pull request is merged, you can safely delete your branch and sync the changes from the main (upstream) repository:

- Delete the remote branch on GitHub either through the GitHub web UI or your local shell as follows:

```
git push origin --delete my-fix-branch
```

- Check out the master branch:

```
git checkout develop -f
```

- Delete the local branch:

```
git branch -D my-fix-branch
```

- Update your master with the latest upstream version:

```
git pull --ff upstream develop
```