Manual of *detonationFoam* solver

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Contents

Abstract

detonationFoam is an open-source solver which can accurately and efficiently simulate compressible, multi-component reactive flow and detonation processes. It is developed based on the OpenFOAM framework. This manual provides a summary of the governing equations and model. Besides, the detailed on how to install and use the solver are provided together with several testing cases.

1. Governing equations and models

The conservation equations for unsteady, compressible, multi-component reactive flow are solved in *detonationFoam*. The governing equations for mass, momentum, energy and species are [1]

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho V) = 0 \tag{1}$$

$$\frac{\partial (\rho V)}{\partial t} + \nabla \cdot (\rho V V) = -\nabla P + \nabla \cdot \tau \tag{2}$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot [(\rho E + P) V] = -\nabla \cdot q + \nabla \cdot (V \cdot \tau) \tag{3}$$

$$\frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot [\rho (V + V_k^{'}) Y_k] = \omega_k \qquad k = 1, ..., N_S - 1 \tag{4}$$

Here ρ is the density of the mixture, $V = (u, v, w)$ is the velocity vector, and P is the pressure. Y_k, $V_k^{'}$ and ω_k are respectively the mass fraction, diffusion velocity and production rate of the *k-th* species. N_S is the total number of the species. The viscous stress is

$$\tau = \mu \left[\nabla V + (\nabla V)^T - \frac{2}{3} I (\nabla \cdot V) \right] \tag{5}$$

in which μ is the dynamic viscosity of the mixture and I is unit tensor.

We assume that the mixture is ideal gas and the equation of state is:

$$P = \frac{\rho R T}{\overline{W}} \tag{6}$$

where T is the temperature, R = 8.314 J/(mole·K) is the universal gas constant, and $\overline{W}$ is the mean molar weight of the mixture.

The total energy E and heat flux q in Eq. (3) are

$$q = -\lambda \nabla T + \rho \sum_{k=1}^{N_S} \left(Y_k h_k V_k^{'} \right) \tag{7}$$

$$E = -\frac{P}{\rho} + \frac{V^2}{2} + \sum_{k=1}^{N_S} \left(Y_k h_k \right) \tag{8}$$

where λ is the thermal conductivity of the mixture, and h_k is the enthalpy of the *k-th* species. The thermodynamic properties of each species are evaluated with *JANAF* polynomials [2]. The enthalpy, h_k, and the specific heat capacity at constant pressure, $C_{p,k}$ of the *k-th* species are:

$$\frac{h_k}{RT} = \sum_{n=0}^{4} \frac{a_{n,k} T^n}{n+1} + \frac{a_{n,5}}{T} \tag{9}$$

$$\frac{C_{p,k}}{R} = \sum_{n=0}^{4} a_{n,k} T^n \tag{10}$$

where $a_{n,k}$ with n = 1~5 are the coefficients for the *k-th* species.

The mixture-averaged transport model provided by Dasgupta et al. [3] is modified and incorporated into *detonationFoam*. The Wilke formula [4, 5] is used to calculate the dynamic viscosity of the mixture:

$$\mu = \sum_{k=1}^{N_S} \frac{X_k \mu_k}{\sum_{j=1}^{N_S} X_j \Phi_{kj}} \tag{11}$$

where X_k is the mole fraction and μ_k is the dynamic viscosity coefficient of the *k-th* species. Φ_{kj} is the dimensionless partition function defined as [5]:

$$\Phi_{kj} = \frac{1}{\sqrt{8}} \left(1 + \frac{W_k}{W_j}\right)^{-\frac{1}{2}} \left[1 + \left(\frac{\mu_k}{\mu_j}\right)^{\frac{1}{2}} \left(\frac{W_j}{W_k}\right)^{\frac{1}{4}}\right]^2 \tag{12}$$

where W_k is the molecule weight of the *k-th* species.

The thermal conductivity of the mixture is obtained from the following formula [6]

$$\lambda = \frac{1}{2} \left(\sum_{k=1}^{N_S} X_k \lambda_k + \frac{1}{\sum_{k=1}^{N_S} \frac{X_k}{\lambda_k}} \right) \tag{13}$$

where λ_k is the thermal conductivity of the *k-th* species.

The diffusion velocity, $V_k^{'}$ in Eq. (4), consists of three parts [7]

$$V_k^{'} = V_{k,Y}^{'} + V_{k,T}^{'} + V_{k,C}^{'} \tag{14}$$

where $V_{k,Y}^{'}$ is the ordinary diffusion velocity and $V_{k,T}^{'}$ is the thermal diffusion velocity. The expressions for $V_{k,Y}^{'}$ and $V_{k,T}^{'}$ are:

$$V_{k,Y}^{'} = -\frac{D_{km}}{X_k} \frac{\partial X_k}{\partial x_i} \tag{15}$$

$$V_{k,T}^{'} = -\frac{D_{km} \Theta_k}{X_k} \frac{1}{T} \frac{\partial T}{\partial x_i} \tag{16}$$

where D_{km} is the mixture-averaged mass diffusion coefficient and Θ_k is the thermal diffusion ratio of the *k-th* species.

The correction velocity, $V_{k,C}^{'}$, is introduced to ensure the compatibility between the species mass conservation and the total mass conservation [1]. It is determined according to the following requirement:

$$\sum_{k=1}^{N_S}\left(\rho Y_k V_k^{'}\right)=0 \tag{17}$$

In *detonationFoam*, the detailed kinetic model can be considered. For a kinetic model containing N_S species, the N_R elementary reactions can be written as [8]

$$\sum_{k=1}^{N_S}(\nu_{k,j}^{'}M_k)\underset{K_{b,j}}{\overset{K_{f,j}}{\Leftrightarrow}}\sum_{k=1}^{N_S}(\nu_{k,j}^{''}M_k)\qquad j=1,...,N_R \tag{18}$$

Here M_k represents the molecular formula for the *k-th* species. $\nu_{k,j}^{'}$ and $\nu_{k,j}^{''}$ are the stoichiometric coefficients of the *k-th* species in the *j-th* elementary reaction. $K_{f,j}$ and $K_{b,j}$ respectively represent the forward and backward reaction rate constants of the *j-th* elementary reaction. The production rate of the *k-th* species can be expressed as [8]

$$\omega_k=W_k\sum_{j=1}^{N_R}[(\nu_{k,j}^{''}-\nu_{k,j}^{'})(K_{f,j}\prod_{k=1}^{N_S}C_k^{\nu_{k,j}^{'}}-K_{b,j}\prod_{k=1}^{N_S}C_k^{\nu_{k,j}^{''}})] \tag{19}$$

where C_k is the molar concentration of the *k-th* species. The reaction rate constant, $K_{f,j}$, can be written in the Arrhenius Law [8] as

$$K_{f,j}=A_jT^{\beta_j}\exp(-\frac{E_{a,j}}{RT}) \tag{20}$$

Here A_j, β_j and $E_{a,j}$ are respectively the pre-exponential factor, temperature exponent and activation energy of the *j-th* forward reaction. The backward reaction rate, $K_{b,j}$, can be evaluated based on $K_{f,j}$ and the equilibrium constant of the *j-th* elementary reaction [8].

2. Compiling the libraries and applications

detonationFoam consists of the Euler equations solver, *detonationEulerFoam*, and the N-S equations solver, *detonationNSFoam*. The framework of the procedure is described in Fig. 1. Depending on the diffusion model used, *detonationNSFoam* is divided into *detonationNSFoam_mixtureAverage* and *detonationNSFoam_Sutherland*.

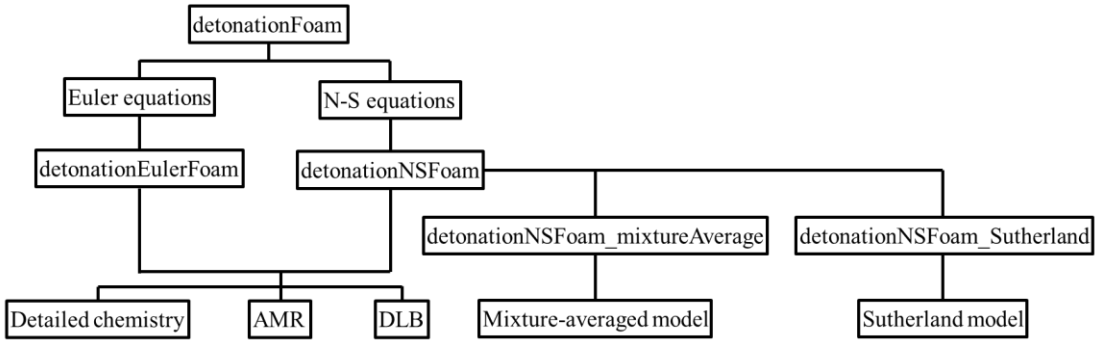

Fig. 1 The framework of the *detonationFoam* solver.

The user can install the program according to the following steps:

1. The solver, *detonationFoam*, is developed based on OpenFOAM V6 [9]. Before installing the solver, please ensure you have installed OpenFOAM V6. Please refer to https://openfoam.org/download/6-ubuntu.

2. Compiling *detonationFoam*.
   - cd applications/solvers/detonationFoam
   - ./Allwmake

3. Example cases

Note: If you want to use the detonationNSFoam_mixtureAverage solver, please use ANSYS CHEMKIN to fit the transport data of Chemkin format. The tran.out can be outputted when you select to process Transport properties with Fit with Verbose Output. Mode detailed steps can be found in https://github.com/ZSHtju/reactingDNS_OpenFOAM.

3.1 1D laminar flame (detonationNSFoam_mixtureAverage)

The 1D premixed laminar flame tutorial is located in /detonationFoam/tutorials/1D_flame. The mixture is stoichiometric H_2/air mixture at 1 atm and 300 K. The user can run the tutorial using the *Allrun* script in /detonationFoam/tutorials/1D_flame. The steady mass fraction of OH and temperature distributions are plotted in Fig. 2.

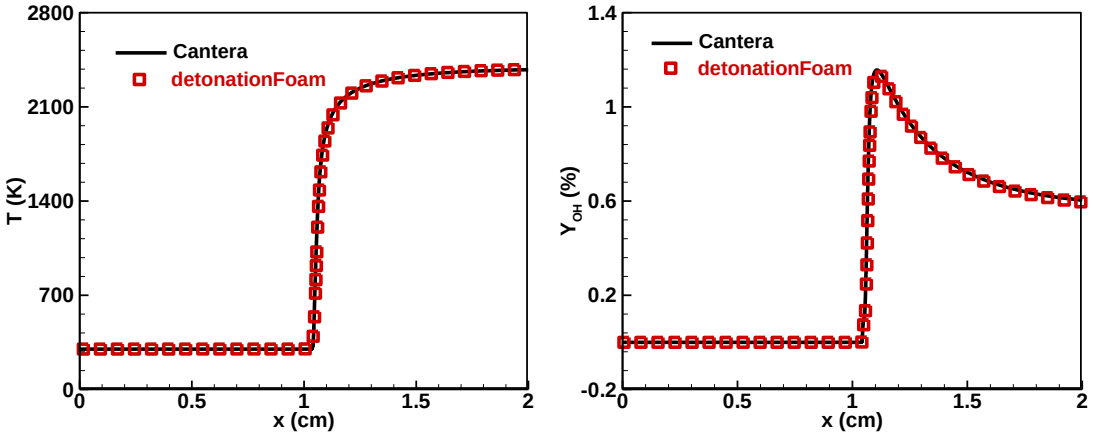

Fig. 2 The steady mass fraction of OH and temperature distributions of the 1D premixed laminar flame.

3.2 1D detonation (detonationNSFoam_Sutherland)

The 1D detonation tutorial is located in /detonationFoam/tutorials/1D_detonation. The initial field is described as follows: the H_2/air mixture with pressure, p = 90 atm, and temperature, T = 3000 K, is set in the region $0 < x < 2$ mm to initiate the detonation. The remaining region is the stoichiometric H_2/air mixture with pressure, p = 1 atm, and temperature, T = 300 K. The uniform grid size used in this case is 5 μm. The user can run the tutorial using the *Allrun* script in /detonationFoam/tutorials/1D_detonation. The temporal pressure and temperature distributions are plotted in Fig. 3.

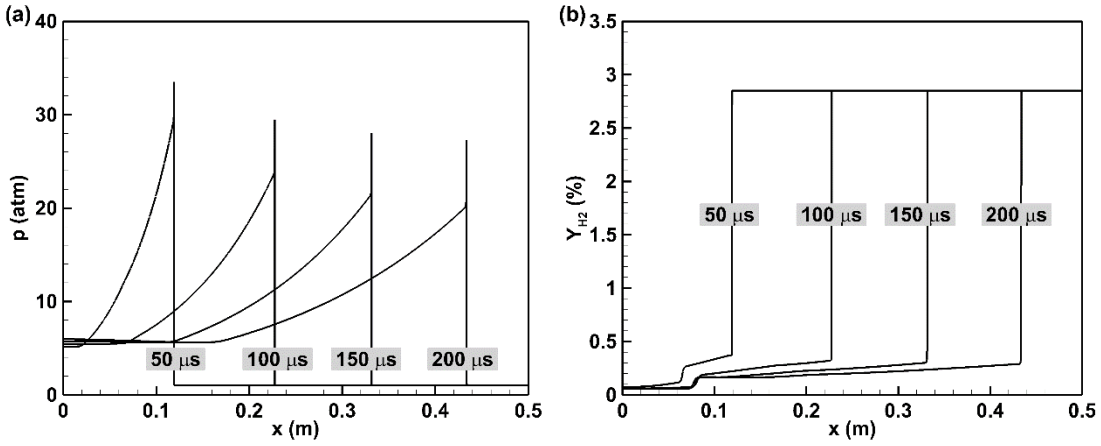

Fig. 3 The temporal pressure and OH mass fraction distributions of the 1D detonation wave.

3.3 2D cellular detonation (detonationNSFoam_Sutherland)

The two-dimensional cellular detonation wave for stoichiometric H_2/O_2 mixtures with p = 8 kPa and T = 300 K is calculated. The basic grid size in this case is 200 μm and four-layer adaptive refinement mesh are used. The initial field settings can be checked in /detonationFoam/tutorials/2D_detonation/0. The user can run the tutorial using the *Allrun* script in /detonationFoam/tutorials/2D_detonation and the simulation results are described in Fig. 4.

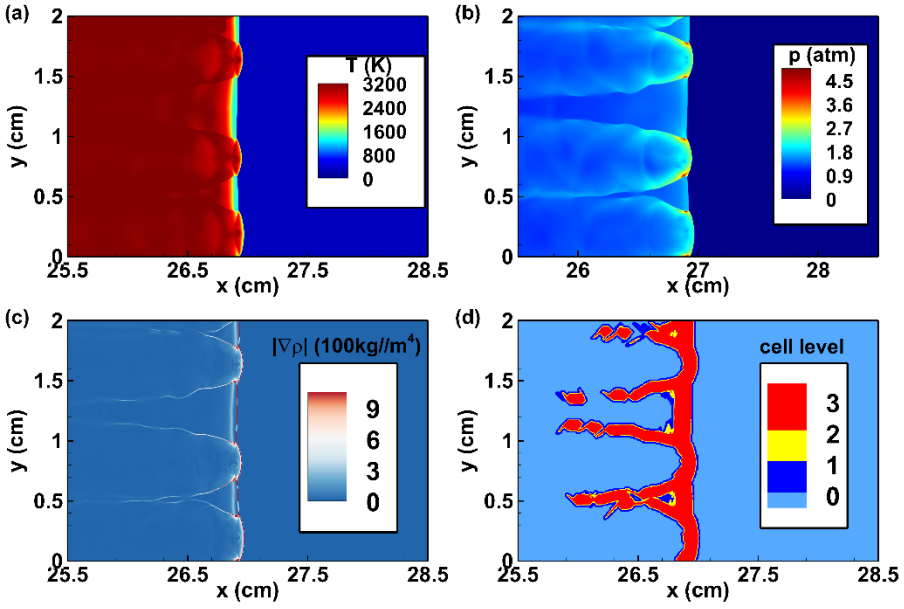

Fig. 4 The contours for (a) temperature, (b) pressure, (c) density gradient and (d) mesh level at t = 100 μs for 2D cellular detonation wave.

References

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