An Eulerian stochastic fields (ESF) method for large eddy simulation of turbulent combustion in compressible flow

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Motivation and introduction

• Eulerian stochastic fields (ESF) is a Monte-Carlo method to solve the transported pdf equations in Eulerian frame.
  – It is easy to coupled with convectional CFD code;
  – It has been used in different combustions, e.g., premixed/non-premixed jet flame, spray combustions.

• ESF method has only been coupled with pressure based solver.
  – Pressure-velocity coupled using SIMPLE or PISO type method;
  – Energy is solved in stochastic fields with neglecting the exchange with kinetic energy;
  – Usage is Limited in low speed conditions (Ma<0.3)
Motivation and introduction

High speed jet flame

Supersonic combustion


Bo Zhou et al., combust. Flame, 2015
Compressible LES solver

Transported equations

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho \hat{u}_j}{\partial x_j} &= 0 \\
\frac{\partial \rho \hat{u}_i}{\partial t} + \frac{\partial (\rho \hat{u}_i \hat{u}_j + \bar{p} \delta_{ij})}{\partial x_j} &= \frac{\partial (\tau_{i,j} - \tau_{ij}^{s gs})}{\partial x_j} \\
\frac{\partial \rho \hat{E}}{\partial t} + \frac{\partial (\rho \hat{E} \hat{u}_j + \bar{p} \hat{u}_j)}{\partial x_j} &= \frac{\partial}{\partial x_j} \left( \hat{u}_j \tau_{i,j} + \rho \nu \frac{\partial k_{ij}^{s gs}}{\partial x_j} + \tilde{q}_j - H_j^{s gs} + \sigma_{ij}^{s gs} \right)
\end{align*}
\]

Total energy

\[
\rho \hat{E} = \rho \hat{e} + \frac{1}{2} \rho \hat{u}_i \hat{u}_i + \rho k_{ij}^{s gs}
\]

Unclosed terms:

\[
\tau_{ij}^{s gs} = \rho u_i u_j - \rho \hat{u}_i \hat{u}_j \\
H_j^{s gs} = \left( \rho E u_j - \rho \hat{E} \hat{u}_j \right) + \left( \rho u_j - \rho \hat{u}_j \right)
\]

Molecular heat flux (unity Lewis number)

\[
\tilde{q}_j = \rho \left( \frac{\nu}{Pr} \frac{\partial \tilde{h}}{\partial x_j} \right)
\]

\[
\sigma_{ij}^{s gs} = u_j \tau_{i,j} - \tilde{u}_j \tau_{i,j}
\]
Compressible LES solver

Sub-grid scale models

\[
\frac{\partial \bar{\rho}k^{sgs}}{\partial t} + \frac{\partial \bar{\rho}k^{sgs} \bar{u}_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\rho v_t}{Pr} \frac{\partial k^{sgs}}{\partial x_j} \right) - \tau_{ij}^{sgs} \frac{\partial \bar{u}_j}{\partial x_j} - c_d \frac{\bar{\rho}}{\bar{\Delta}} (k^{sgs})^{3/2}
\]

\[
\nu_t = c_\mu \bar{\Delta} \sqrt{k^{sgs}}
\]

Closure for momentum equation

\[
\tau_{ij}^{sgs} = -2\bar{\rho} v_t \left( \bar{\delta}_{ij} - \frac{1}{3} \bar{\delta}_{kk} \delta_{ij} \right) + \frac{2}{3} \bar{\rho} k^{sgs} \delta_{ij}
\]

Closure for energy equation

\[
-H_j^{sgs} + \sigma_{ij}^{sgs} = \rho \frac{v_t}{Pr} \left( \frac{\partial \bar{h}}{\partial x} + \bar{u}_i \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial k^{sgs}}{\partial x_j} \right)
\]
Eulerian stochastic fields method

Joint pdf equation

\[
\frac{\partial \tilde{P}_{sgs}(\psi)}{\partial t} + \bar{\rho} \tilde{u}_j \frac{\partial \tilde{P}_{sgs}(\psi)}{\partial x_j} + \sum_{n=1}^{N_s} \frac{\partial}{\partial \psi_{\alpha}} \left[ \bar{\rho} \tilde{\omega}_{\alpha}(\psi) \tilde{P}_{sgs}(\psi) \right] = \frac{\partial}{\partial x_i} \left[ \frac{(\mu + \mu_{sgs})}{\sigma_{sgs}} \frac{\partial \tilde{P}_{sgs}(\psi)}{\partial x_i} \right] - \frac{C_d}{\tau_{sgs}} \sum_{n=1}^{N} \frac{\partial}{\partial \psi_{\alpha}} \left[ \bar{\rho}(\psi_{\alpha} - \phi_{\alpha}(x, t)) \tilde{P}_{sgs}(\psi) \right]
\]

Impossible to solve directly due to the Multi-dimensions \((N_s + 5)\). Usually, it is solved using Monte-Carlo approaches.

ESF method

\[
\tilde{P}_{sgs}(\psi; x, t) = \frac{1}{N} \sum_{n=1}^{N} \left[ \prod_{n=1}^{N_s} \delta (\psi_{\alpha} - \xi_{\alpha}^n) \right] \\
\tilde{\phi}_{\alpha} = \frac{1}{N} \sum_{n=1}^{N} \xi_{\alpha}^n \\
\bar{\rho} d\xi_{\alpha}^n = -\bar{\rho} \tilde{u}_j \frac{\partial \xi_{\alpha}^n}{\partial x_j} dt + \frac{\partial}{\partial x_i} \left( \Gamma_t \frac{\partial \xi_{\alpha}^n}{\partial x_i} \right) dt + \bar{\rho} \tilde{\omega}_{\alpha}(\psi_{\alpha}^n) dt \\
- \frac{1}{2} \frac{\bar{\rho}}{\tau_{sgs}} \left( \xi_{\alpha}^n - \tilde{\phi}_{\alpha} \right) dt + \bar{\rho} \sqrt{2 \Gamma_t \frac{\partial \xi_{\alpha}^n}{\partial x_i}} dW_i^n,
\]
Numerical implementation

LES equations

The LES solver is a modified version of rhoCentralFoam in OpenFOAM. The convective terms of the equations are discreted using the Kurganov and Tadmor scheme.

ESF equations

Step 1: Advection-diffusion-Wiener

\[ \rho \frac{\partial \xi^n}{\partial t} = \ell_{ad}(\xi^n) + \ell_{wien}(\xi^n) + \ell_{mix}(\xi^n, \widetilde{\phi}) + \rho \dot{\omega}(\psi^n) \]

Step 2: Micro-mixing

\[ \xi_{\alpha}^{n(2)} = \xi_{\alpha}^{n(1)} - 0.5 C_{\phi} \frac{\Delta t}{\tau_{sgs}} (\xi_{\alpha}^{n(2)} - \phi_{\alpha}^{(1)}) \]

Step 3: Energy correction

\[ h^{n(3)} = h^{n(2)} + \left( \hat{h} - \frac{1}{N} \sum_{m=1}^{N} h^{m(2)} \right) \]

Step 4: Chemical reaction

\[ \xi_{\alpha}^{n} t_{n+1} = \xi_{\alpha}^{n(3)} + \int_{0}^{\Delta t} \dot{\omega}(\psi) dt, \quad t = 0: \psi = \psi^{n(3)} \]
Validation case

Table I Inflow conditions of the air stream and the hydrogen jet

<table>
<thead>
<tr>
<th></th>
<th>Ma</th>
<th>T(K)</th>
<th>P(MPa)</th>
<th>ρ(kg/m³)</th>
<th>Y_{O_2}</th>
<th>Y_{N_2}</th>
<th>Y_{H_2O}</th>
<th>Y_{H_2}</th>
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<td>0.1</td>
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<td>0.736</td>
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<td>0.097</td>
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<td>0</td>
<td>0</td>
<td>1</td>
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</tbody>
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Non-reacting flow field
Reacting flow field

Time average during 1.2 ms, with NF=8, Cphi=2.0
Flame stabilization

Two pairs of recirculation zones:
1) Induced by the fuel injection;
2) Induced by the strut.

The flame is stabilized by the strut induced recirculation zones.

Local extinction/re-ignition behavior around the fuel injection induced recirculation zones.
Most previous studies failed to predict the temperature profile close to the strut \((x=11\, \text{mm})\);

The ESF method provide good agreement at \(x=11\, \text{mm}\), which reveals that the ESF can capture the local extinction/re-ignition behavior, successfully.
Conclusions

• The Eulerian stochastic fields method was implemented to a compressible LES solver in OpenFOAM;

• The LES-ESF solver was validated on the strut-stabilized combustion in a supersonic combustor;
  – The compressible LES solver provide good performance on the supersonic flow field;
  – Comparing to the WSR model, the ESF method can provide much better prediction for the local extinction and re-ignition behavior in the present condition.
Thanks for your attention