The explicit filtering method for large eddy simulations of a turbulent premixed flame

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Introduction

- Combustors operate in *lean premixed regime* to minimize pollutant emissions.
  - High *Re* flows, large range of energetic flow scales
  - Thin reaction zone (TRZ)

- Large Eddy Simulations of complex turbulent reacting flows
  - Capture dynamics of large flow structures and their interactions with flames

- Explicit filtering approach of LES (EFLES) is based on approximate deconvolution modelling (ADM).
  - Mathew et. al, *Phys. Fluids* 15 (8) (2003).
  - Applied successfully to non-reacting flow computations

Formulation

- Governing Eq. for fully compressible, multi-component reacting flow in conservative form,

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}_i(\mathbf{U})}{\partial x_i} = \frac{\partial \mathbf{F}_{v,i}(\mathbf{U})}{\partial x_i} + \mathbf{S}(\mathbf{U}), \tag{1}$$

$\mathbf{U} = [\rho\ \rho u\ \rho v\ \rho w\ \rho e\ \rho Y_1 \ldots \rho Y_N]^T$, $\mathbf{S} = [0\ 0\ 0\ 0\ 0\ \dot{\omega}_1 \ldots \dot{\omega}_N]^T$.

- Eq. for LES field, $\overline{\mathbf{U}} = G * \mathbf{U}$,

$$\frac{\partial \overline{\mathbf{U}}}{\partial t} + \frac{\partial \mathbf{F}_i(\overline{\mathbf{U}})}{\partial x_i} = \frac{\partial \mathbf{F}_{v,i}(\overline{\mathbf{U}})}{\partial x_i} + \mathbf{S}(\overline{\mathbf{U}}) + \underbrace{\mathcal{R}(\mathbf{U}, \overline{\mathbf{U}}) + \mathcal{R}_S(\mathbf{U}, \overline{\mathbf{U}})}_{remainder\ terms}.$$

  - G - low pass spatial filter.

Formulation

- **ADM** uses $\mathbf{U} \approx \mathbf{U}^* = Q * \overline{\mathbf{U}}$ to get, $\quad [Q \approx G^{-1}]$

$$\frac{\partial \overline{\mathbf{U}}}{\partial t} = G * \left\{ -\frac{\partial \mathbf{F}_i(\mathbf{U}^*)}{\partial x_i} + \frac{\partial \mathbf{F}_{v,i}(\mathbf{U}^*)}{\partial x_i} + \mathbf{S}(\mathbf{U}^*) \right\} = G * \mathscr{L}(\mathbf{U}^*),$$

  - Stolz, Adams, *Phys. Fluids* 11 (7) (1999).

- Numerical solution of ADM Eq., with timestep Δt;
  1. Deconvolution: $\mathbf{U}^{*(n)} = Q * \overline{\mathbf{U}}^{(n)}$
  2. Numerical Integration:

$$\overline{\mathbf{U}}^{(n+1)} = \overline{\mathbf{U}}^{(n)} + \Delta t [G * \mathscr{L}(\mathbf{U}^{*(n)})]$$

$$=> \overline{\mathbf{U}}^{(n+1)} = G * [\mathbf{U}^{*(n)} + \Delta t \mathscr{L}(\mathbf{U}^{*(n)})] + \underbrace{[\overline{\mathbf{U}}^{(n)} - G * \mathbf{U}^{*(n)}]}_{neglect\ [\because G*\mathbf{U}^* \approx G*\mathbf{U}]}$$

Formulation

3 stage ADM procedure

1. Deconvolution: $\mathbf{U}^{*(n)} = Q * \overline{\mathbf{U}}^{(n)}$
2. Numerical Integration: $\mathbf{U}^{*(n)} \rightarrow \mathbf{U}^{*(n+1)}$
3. Filtering: $\overline{\mathbf{U}}^{(n+1)} = G * \mathbf{U}^{*(n+1)}$

1. Deconvolution: $\mathbf{U}^{*(n+1)} = Q * \overline{\mathbf{U}}^{(n+1)}$

Combine to an explicit filtering step $E = Q * G$

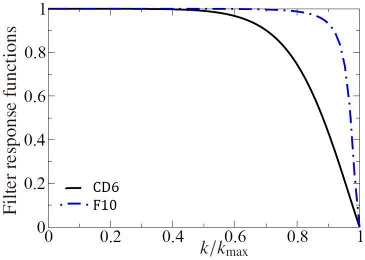
Explicit Filtering LES

1. Numerical Integration: $\mathbf{U}^{*(n)} \rightarrow \mathbf{U}^{*(n+1)}$, (using Eq. (1) in terms of $\mathbf{U}^{*}$)
2. Filtering: Update $\mathbf{U}^{*(n+1)}$ with filtered field $E * \mathbf{U}^{*(n+1)}$

- Mathew et. al, *Phys. Fluids* 15 (8) (2003).

Explicit Filter

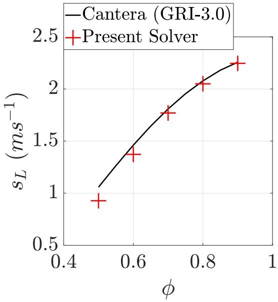
- $E \approx I$ over a range of large computed scales.
- E falls off to zero over a small range of the highest represented wavenumbers.
- As the represented spectral range is increased, EFLES ensures monotonic convergence to DNS.



Response Functions
Mathew, arXiv (2016)

Flow Solver

- Discretization
  - 8^{th} order central difference spatial discretization
  - 3^{rd} order R-K time marching
- Explicit Filtering
  - 10^{th} order spatial filter
- 13 species reduced chemical mechanism
  - Sankaran et. al, *Proc. Combust. Inst.* 31 (1) (2007)
- Navier-Stokes Characteristic Boundary Conditions (NSCBC)
  - Poinsot, Lele, *J. Comp. Phys.* 101 (1) (1992)



Variation of s_L with ϕ for CH_4-air premixed flames (T_u = 800 K, p_0 = 1 atm).

Filter Adaptation

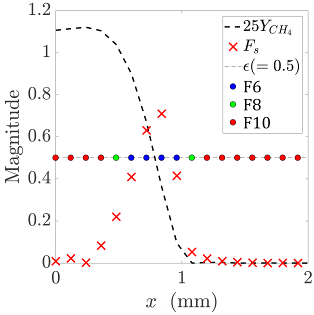
- Steep species gradients are detected using the sensor,

$$F_s = \left[\frac{\delta_F}{|Y_{CH_4,u} - Y_{CH_4,b}|}|\nabla Y_{CH_4}|\right] H\left(5.0 - \frac{\delta_F}{\Delta_{local}}\right).$$

- Progressively reduce filter order to 6 where $F_s \geq 0.5$.
- Adaption is performed along a mesh direction i when

$$\frac{\hat{x}_i.\nabla Y_{CH_4}}{|\nabla Y_{CH_4}|} > \frac{1}{\sqrt{3}}.$$

  - Patel, Mathew, *Fluids* 4 (3) (2019).



Computational Domain

Turbulent premixed CH_4-air round jet flame

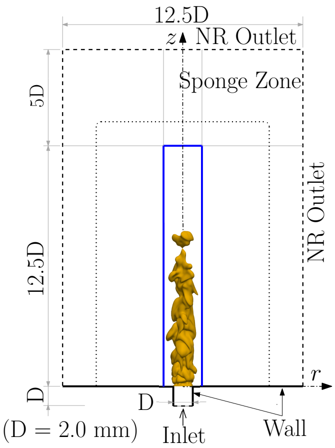
- $\phi = 0.8$, $T_u = 800$ K

Laminar flame properties (from Cantera)

- $s_L = 2.05$ ms^{-1}, $T_b = 2313.65$ K
- $\delta_F = 300\ \mu$m, $\delta_H = 120\ \mu$m

Nominal mesh parameters

	Δ (μm)	δ_F/Δ	δ_H/Δ	Points (x10^6)
DNS	30	10.0	4.0	29.2
LES4x	120	2.5	1.0	1.1
LES6x	180	1.7	0.7	0.5



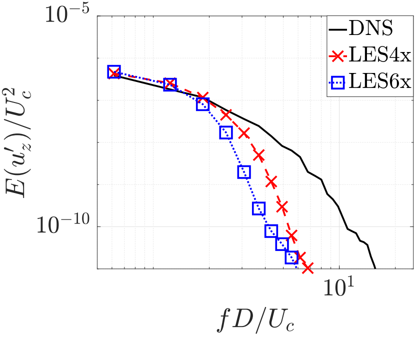
Inflow Conditions

- Top hat mean axial velocity profile
  - $U_c = 65$ ms^{-1}
  - $Re = U_c D/\nu = 1500$

- Inflow turbulence
  - Divergence free synthetic velocity fluctuations
    - Von Karman-Pao energy spectrum
  - Isotropic turbulence boxes are blended to generate a long dataset.
    - Larsson, *J. Comp. Phys.* 228 (2009)
  - Turbulent fluctuations are advected using *Taylor's hypothesis*

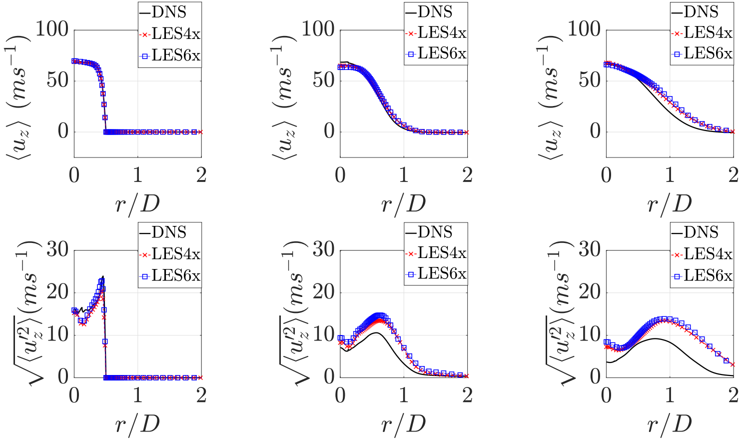
Results: Power Spectral Density

- PSD at low frequencies ($fD/U_c \leq 1$) are the same.
- Filter removes high wavenumber content in two LES cases.
- Monotonic convergence to DNS result is evident.
- Lack of wide intertial range due to low value of Re.



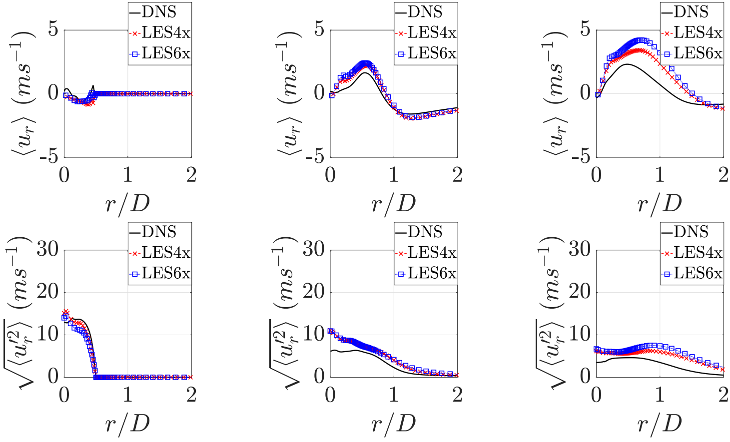
Normalised PSD on centerline at $z/D = 1.0$

Time averaged flow statistics



(a) $z/D = 0.0$ (b) $z/D = 2.0$ (c) $z/D = 5.0$

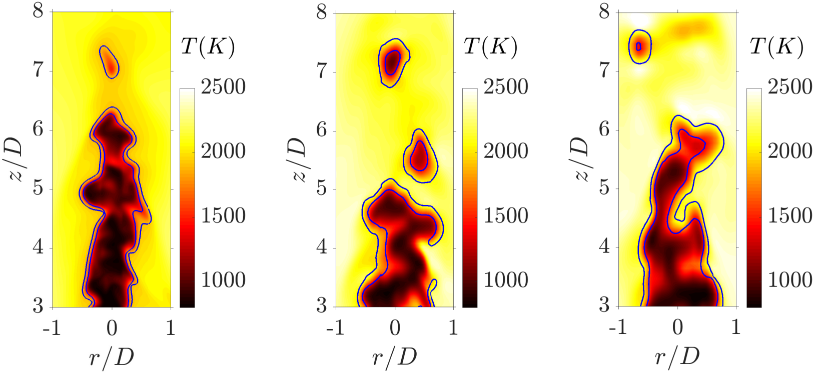
Time averaged statistics of streamwise velocity.



(a) $z/D = 0.0$ (b) $z/D = 2.0$ (c) $z/D = 5.0$

Time averaged statistics of radial velocity.

Instantaneous Snapshots

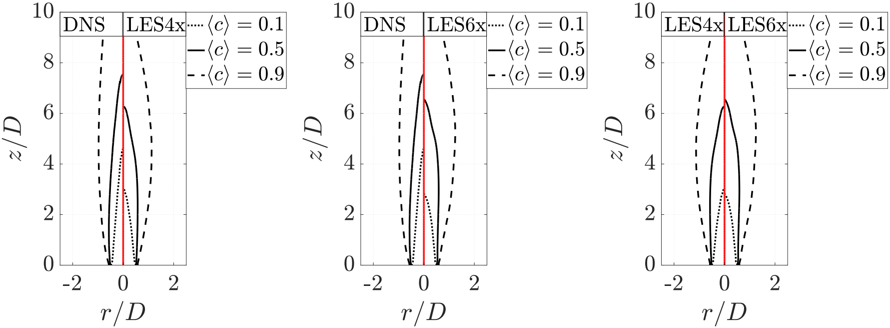


(a) DNS (b) LES4x (c) LES6x

Typical instantaneous snapshots of temperature ($t \approx 4.0 t_{FL}$) with the contour of Heat Release Rate, $\dot{q} = 5.0 \times 10^9$ Js^{-1}.

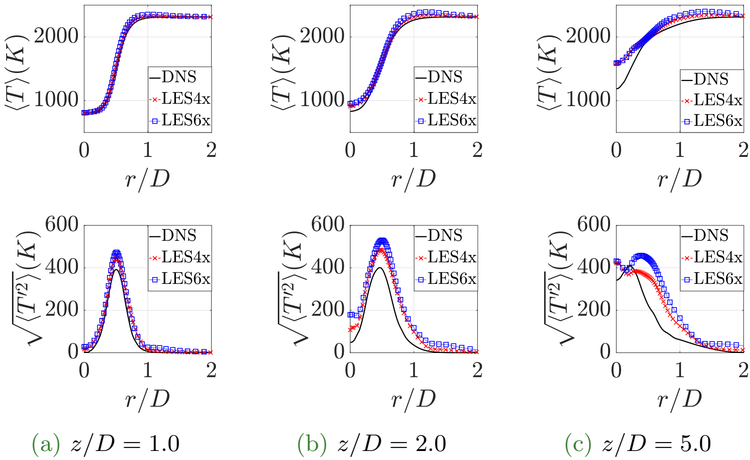
Mean Progress Variable Contours

- Small reduction in mean flame height in EFLES cases.
- LES results show thicker flame brush.



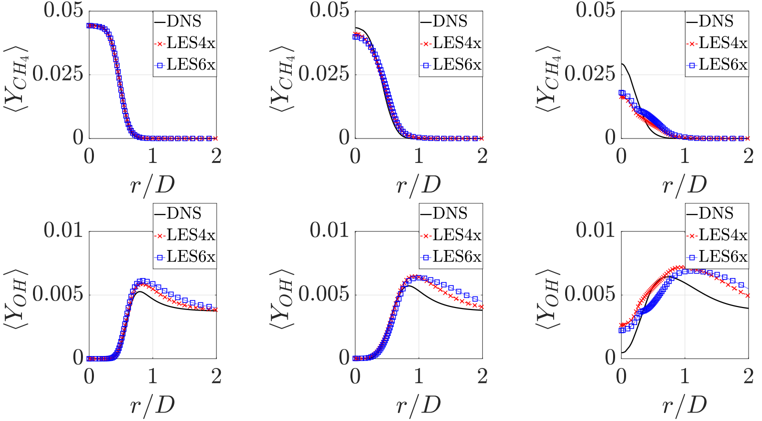
Contours of time averaged progress variable, $\langle c \rangle = \langle Y_{CO_2} \rangle / Y_{CO_2,b}$.

Time averaged statistics



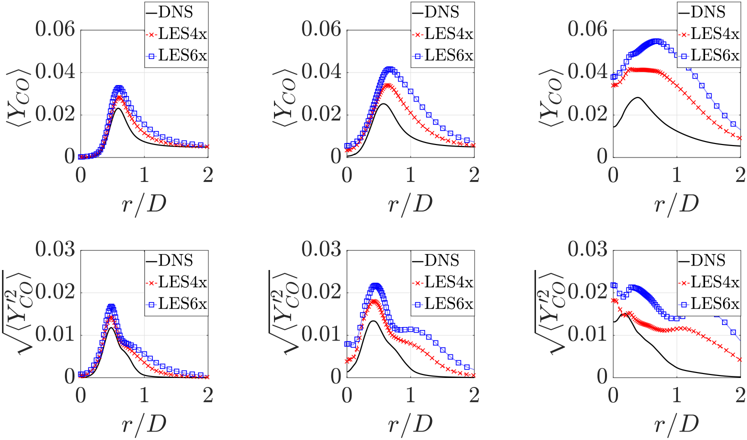
Time averaged statistics of temperature.

Time averaged statistics



(a) $z/D = 1.0$ (b) $z/D = 2.0$ (c) $z/D = 5.0$

Time averaged statistics of CH_4 and OH mass fraction.



(a) $z/D = 1.0$ (b) $z/D = 2.0$ (c) $z/D = 5.0$

Time averaged statistics of CO mass fraction.

Conclusion

- First application of EFLES approach to a simple realistic premixed jet flame configuration.
- LES results for velocity, temperature and major species show good qualitative and quantitative agreement.
- LES predicts a slightly shorter flame height and a moderately thicker flame brush.
- Use of QSS assumptions in present mechanism may lead to large deviations in CO prediction by EFLES computations.
- EFLES is a promising approach for LES of turbulent reacting flow as well.
- At high *Re* flows or when flame length scale is thinner than grid resolution , additional SGS model is needed for reaction rate terms (Ongoing work).