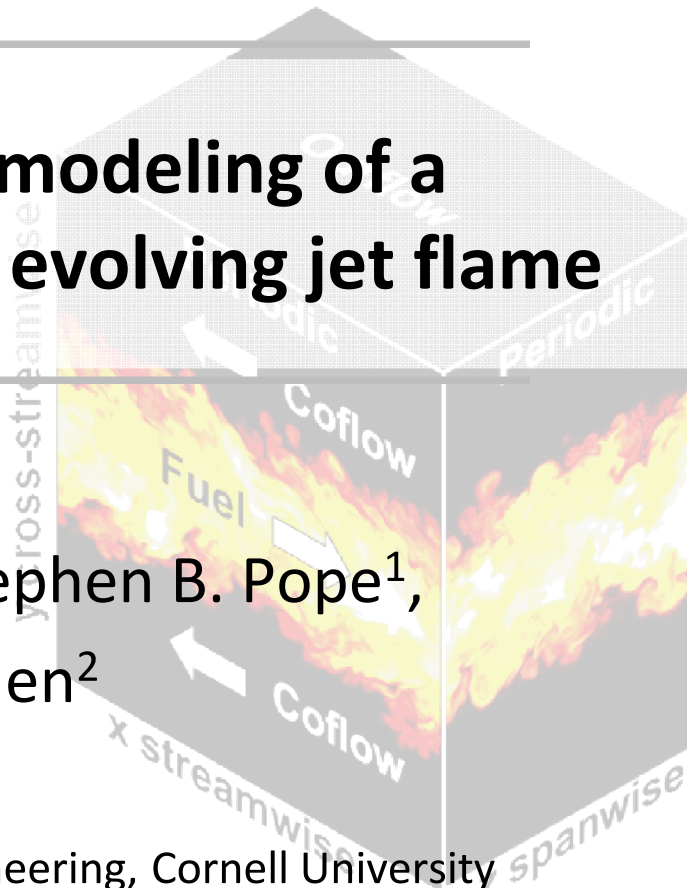
SAND2012-6122C

34th International Symposium on Combustion

August 1, 2012, Warsaw, Poland

Large-eddy simulation/PDF modeling of a non-premixed CO/H_2 temporally evolving jet flame



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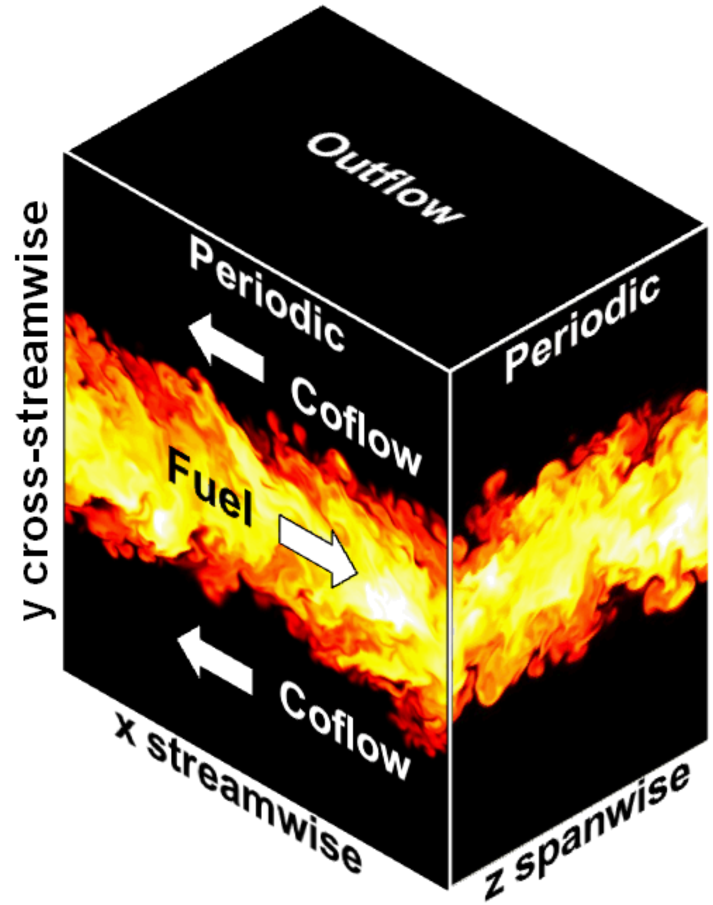
Introduction

- Methodology
  - **Direct numerical simulation** (DNS): CPU hours ~ $O(10^6)$ (Sandia)
  - **Large-eddy simulation/PDF modeling**
    - Flow, turbulence: Large-eddy simulation (LES)
    - Turbulence-chemistry interactions: Probability density function methods (PDF)
- Goal: Computationally-efficient predictive models for turbulent reacting flows
  - Improve the capabilities of LES/PDF by making detailed comparisons with DNS of the same flames and developing advanced SGS models
  - Performance of the LES/PDF will be assessed via *a posteriori* comparisons with DNS in turbulent jet flames
  - Computational speedup to DNS: **factor of 10^3-10^4**

Simulation overview

- Direct numerical simulation (Hawkes *et al.*, 2007)
  - Non-premixed CO/H_2 temporally evolving planar jet flame
  - Re = 2510, 4478, 9079 and Da = 0.011
  - Skeletal mechanism with 11 species
  - Fuel (syngas): 50% CO, 10% H_2, 40% N_2
  - Co-flow: 25% O_2, 75% N_2
  - **500 million** grid points (uniform mesh)

- Large-eddy simulation/PDF modeling
  - Hybrid finite-volume/Monte-Carlo method
  - Same boundary conditions and chemical mechanism as DNS
  - **1 million** grid points (uniform mesh)
  - 20 particles per cell



Schematic of the DNS configurations

Transport equations of PDFs in LES/PDF

- One-point, one-time density-weighted joint PDF of compositions $f(\boldsymbol{\psi};\boldsymbol{x},\boldsymbol{t})$

$$\frac{\partial f}{\partial t} + \nabla \cdot [f(\widetilde{\boldsymbol{u}} + \widetilde{\boldsymbol{u}|\boldsymbol{\psi}})] = -\frac{\partial}{\partial \psi_\alpha}\left[f\left(\frac{1}{\overline{\rho}}\overline{\nabla \cdot (\rho\Gamma_{(\alpha)}\nabla\phi_\alpha)|\boldsymbol{\psi}} + S_\alpha(\boldsymbol{\psi})\right)\right]$$

- Modeling of the **conditional diffusion term** using the IEM model

$$\gamma_\alpha(\boldsymbol{\psi},\boldsymbol{x},t) \equiv \frac{1}{\overline{\rho}}\overline{\nabla \cdot (\rho\Gamma_{(\alpha)}\nabla\phi_\alpha)|\boldsymbol{\psi}}$$

$$\gamma_\alpha(\boldsymbol{\psi},\boldsymbol{x},t) = -\Omega_m(\psi_\alpha - \widetilde{\phi}_\alpha) + \widetilde{\mathcal{D}} \qquad \widetilde{\mathcal{D}} \equiv \frac{1}{\overline{\rho}}\nabla\cdot(\overline{\rho}\Gamma\nabla\widetilde{\phi}) \qquad \Omega_m = C_\phi(\Gamma+\Gamma_T)/\Delta^2$$

Molecular transport — Mixing frequency

- Particle method in LES/PDF

$$d\boldsymbol{X}^*(t) = \left(\widetilde{\boldsymbol{u}} + \frac{\nabla\overline{\rho}\Gamma_T}{\overline{\rho}}\right)^* dt + \sqrt{2\Gamma_T^*}d\boldsymbol{W},$$

$$d\boldsymbol{\phi}^*(t) = -\Omega_m^*(\boldsymbol{\phi}^* - \widetilde{\boldsymbol{\phi}}^*)dt + \widetilde{\mathcal{D}}^*dt + \boldsymbol{S}(\boldsymbol{\phi}^*)dt.$$

Implementation of LES/PDF

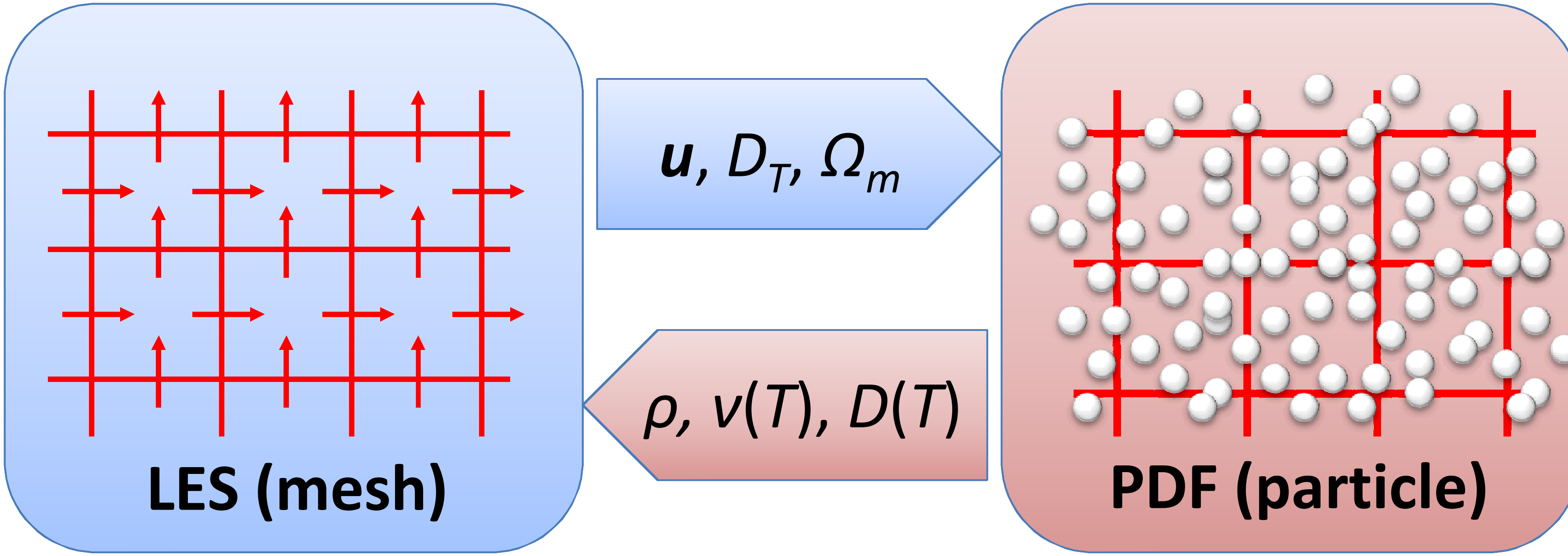
- LES: high-order-accurate LES code ***NGA*** (Desjardins *et al*., 2008)
  - Second-order accuracy in space and time
  - LES filter width $\Delta = 8\Delta_{x,\,\mathrm{DNS}}$
  - Dynamic subgrid-scale model
  - Convective outflow boundary condition

- PDF: highly scalable code ***HPDF*** (Wang and Pope, 2011)
  - Second order accuracy in space and time
  - Two-way coupling of LES/PDF
  - IEM mixing model with molecular transport (Viswanathan *et al*., 2011)

O. Desjardins *et al*, *J. Comput. Phys., 227*, 7125-7159, 2008

H. Wang and S. B. Pope, *Proc. of Combust. Inst.,* 33, 1319-1330, 2011

S. Viswanathan *et al*., *J. Comput. Phys.*, 230, 6916-6957, 2011



- Solve an additional mean specific volume equation to smooth numerical noise in the density field from PDF (Popov *et al.* 2011)

$$\overline{\rho}\frac{\partial \widetilde{v}}{\partial t} + \overline{\rho}\widetilde{\boldsymbol{u}} \cdot \nabla \widetilde{v} = \nabla \cdot (\overline{\rho}(\Gamma + \Gamma_T)\nabla \widetilde{v}) + S_v$$

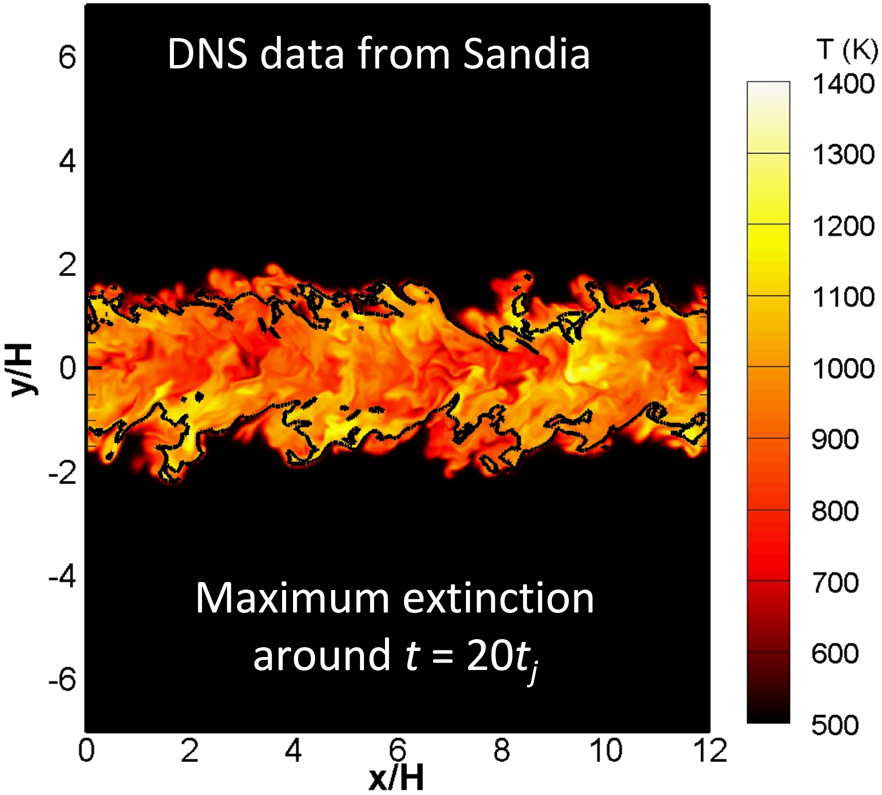
S_v: source term due to the volume expansion (heat release)

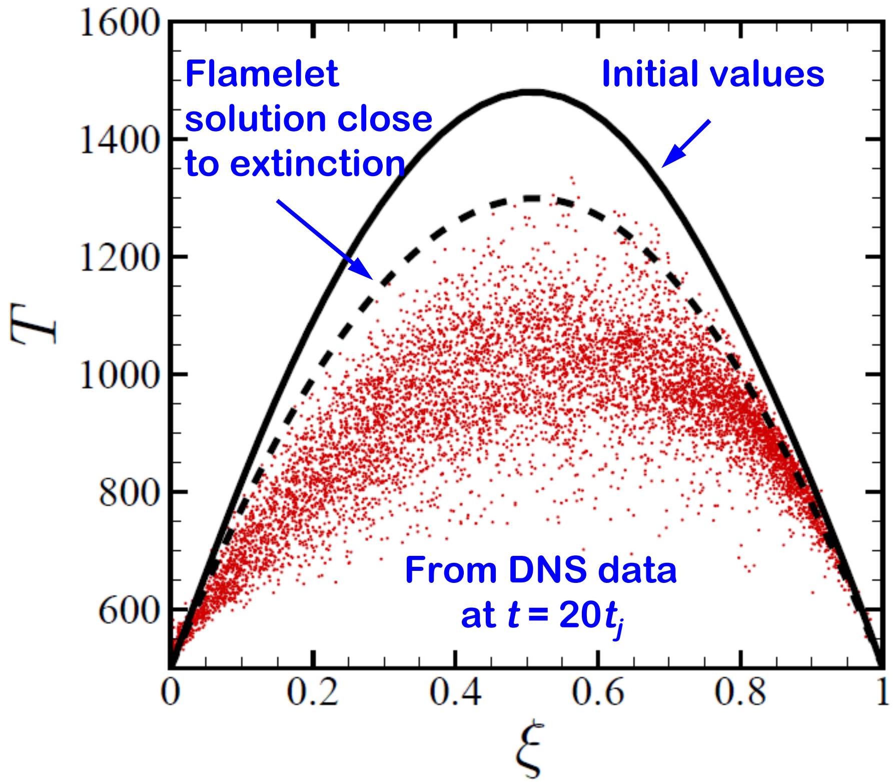
- Transport properties are modeled by empirical formula

$$\mu/\overline{\rho} = \nu_0(\widetilde{T}/T_0)^{1.67} \text{ and } \Gamma = c_0\nu_0(\widetilde{T}/T_0)^{1.77}$$

Turbulence-Chemistry Interactions

- Mixing is initially rapid enough relative to reaction at a low *Da* number
- Strong turbulence-chemistry interactions resulting in local extinction





$t_j = H/U$ with the characteristic jet velocity U and the jet height H

Contour line: stoichiometric mixture fraction

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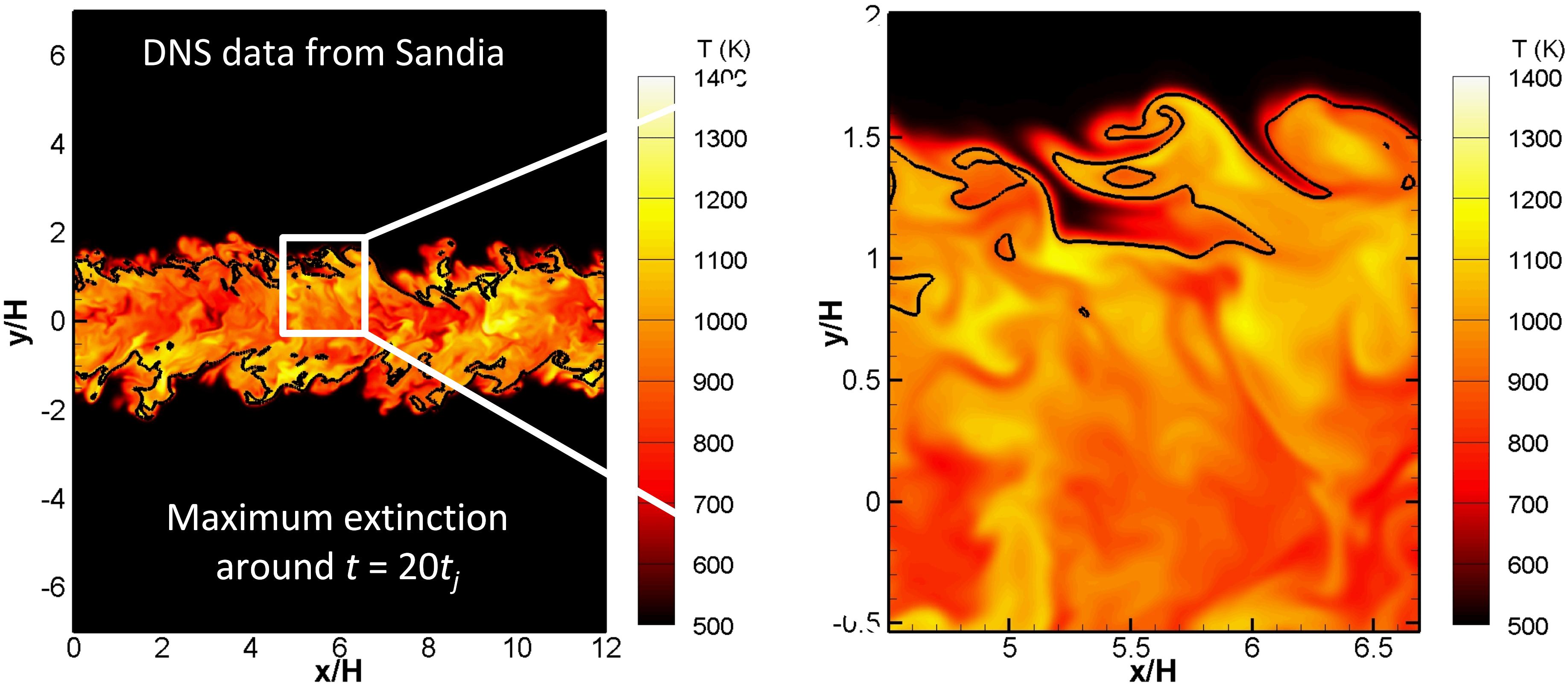
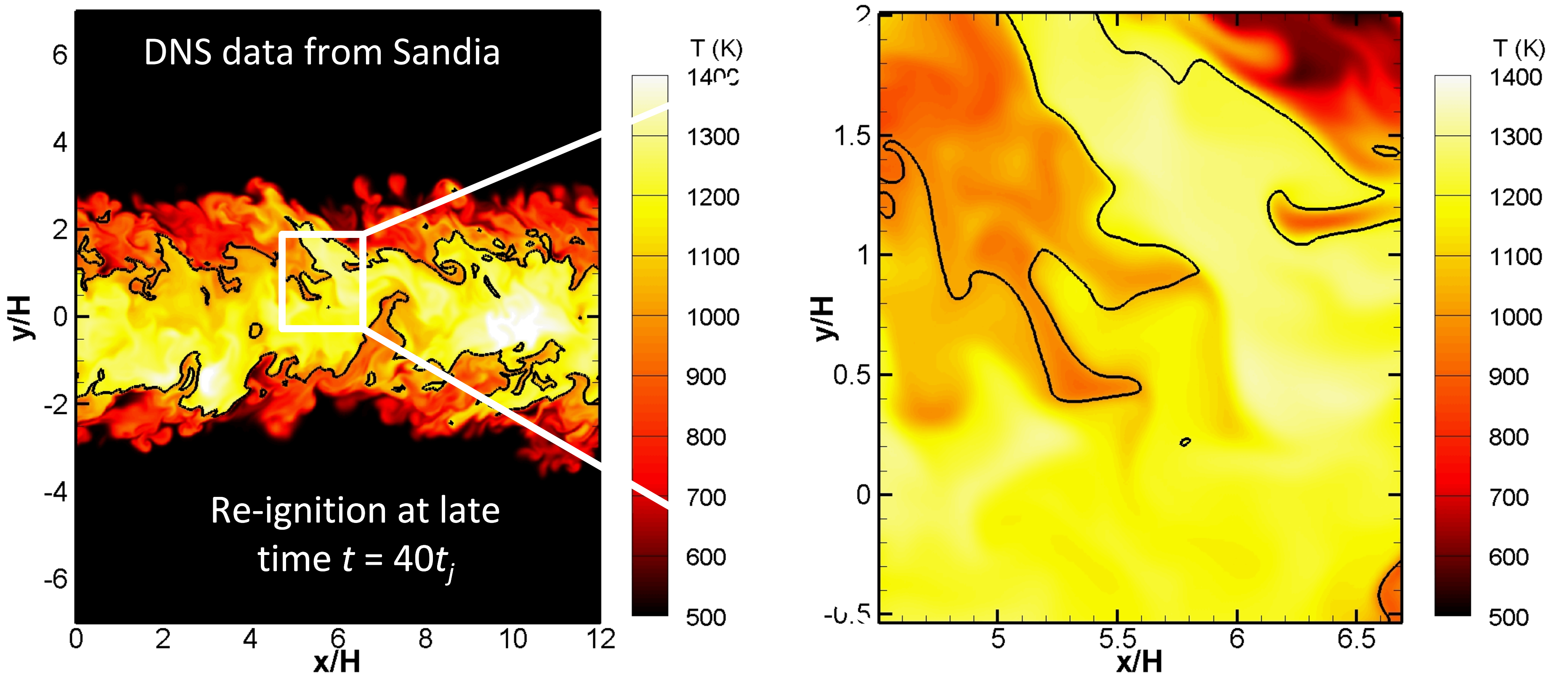


$t_j = H/U$ with the characteristic jet velocity U and the jet height H

Contour line: stoichiometric mixture fraction

Turbulence-Chemistry Interactions

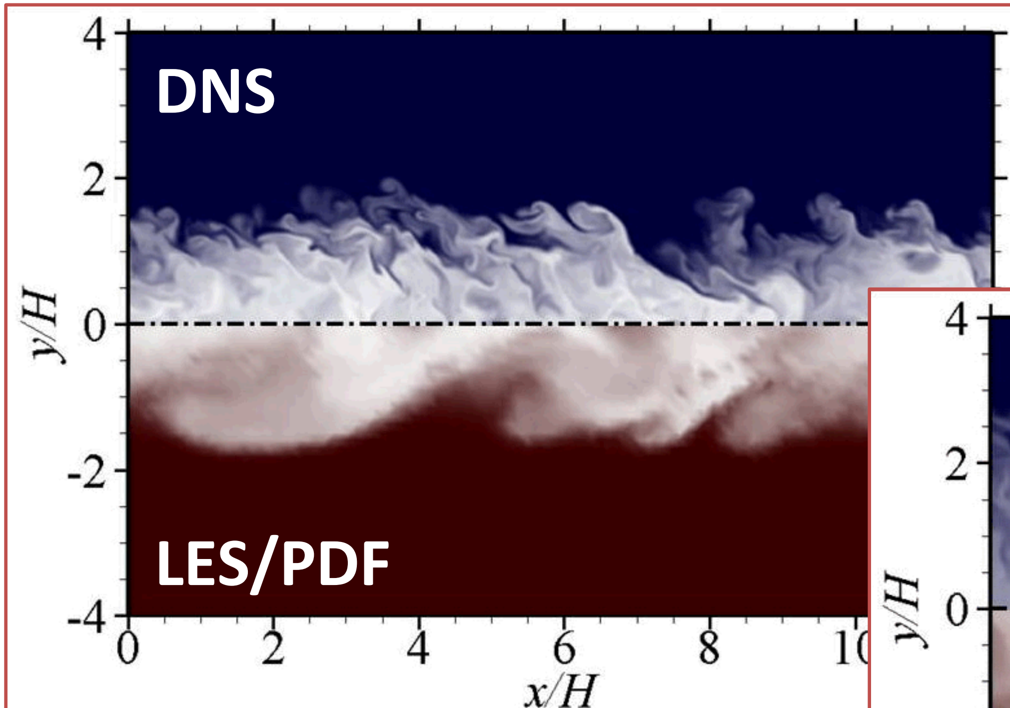
- Strong turbulence-chemistry interactions resulting in local extinction followed by re-ignition



t_j = H/U with the characteristic jet velocity U and the jet height H

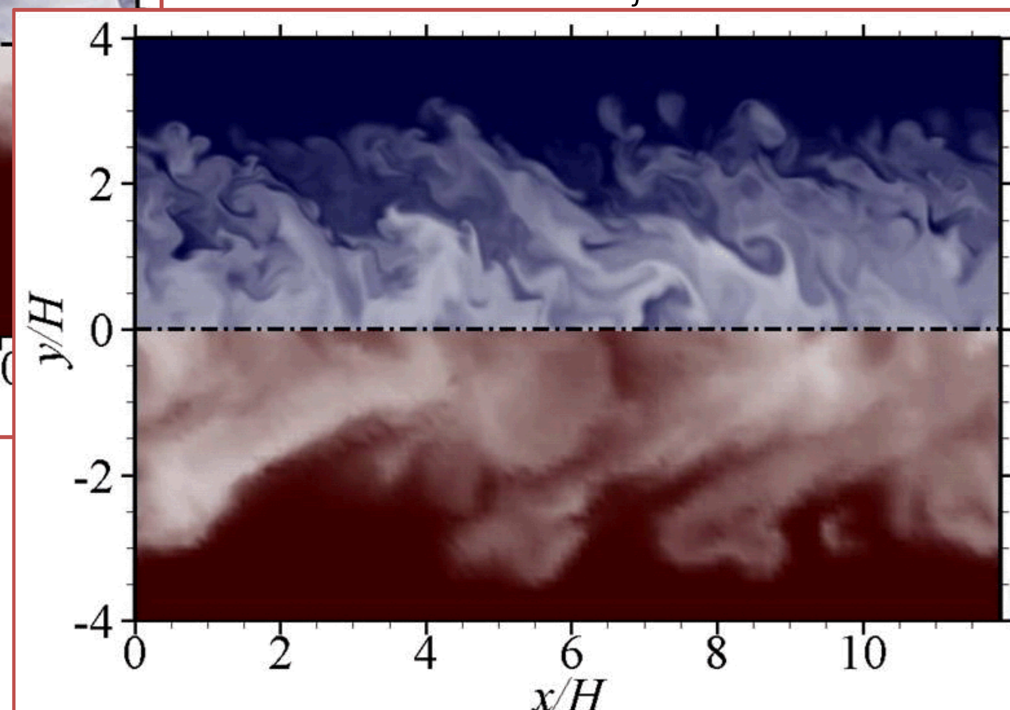
Contour line: stoichiometric mixture fraction

Comparisons between DNS and LES/PDF: Contours of mixture fraction



$t = 20t_j$

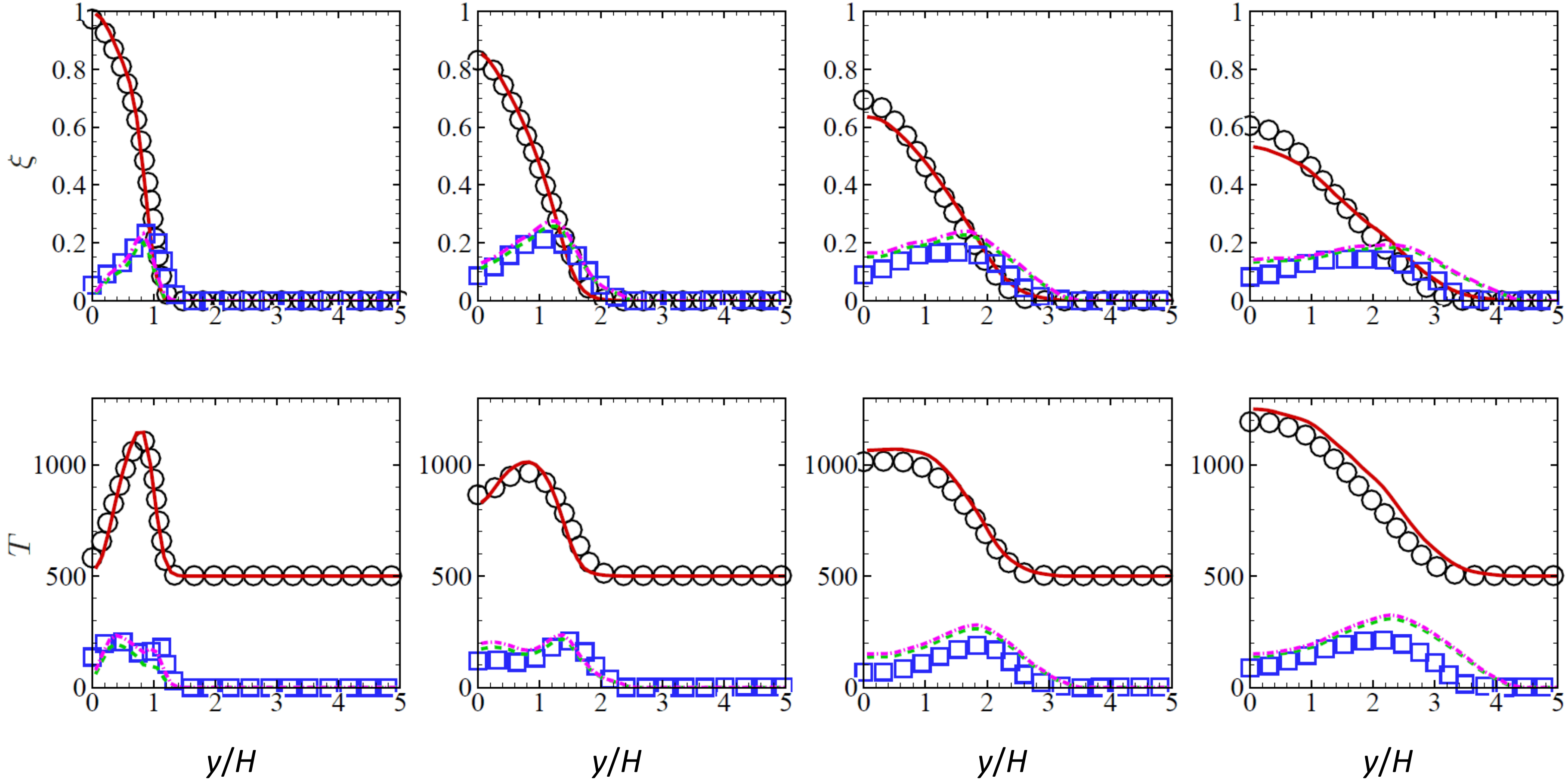
$t = 40t_j$



Re = 9079, DNS: 864 × 1008 × 576 = 501.6M, LES/PDF: 108 × 126 × 72 = 0.98M

Comparisons between DNS and LES/PDF

○: mean in DNS —: mean in LES/PDF
□: rms in DNS ---: resolved rms in LES/PDF -·-: total rms in LES/PDF



$t = 10t_j$ $t = 20t_j$ $t = 30t_j$ $t = 40t_j$

Comparisons between DNS and LES/PDF

○: mean in DNS —: mean in LES/PDF

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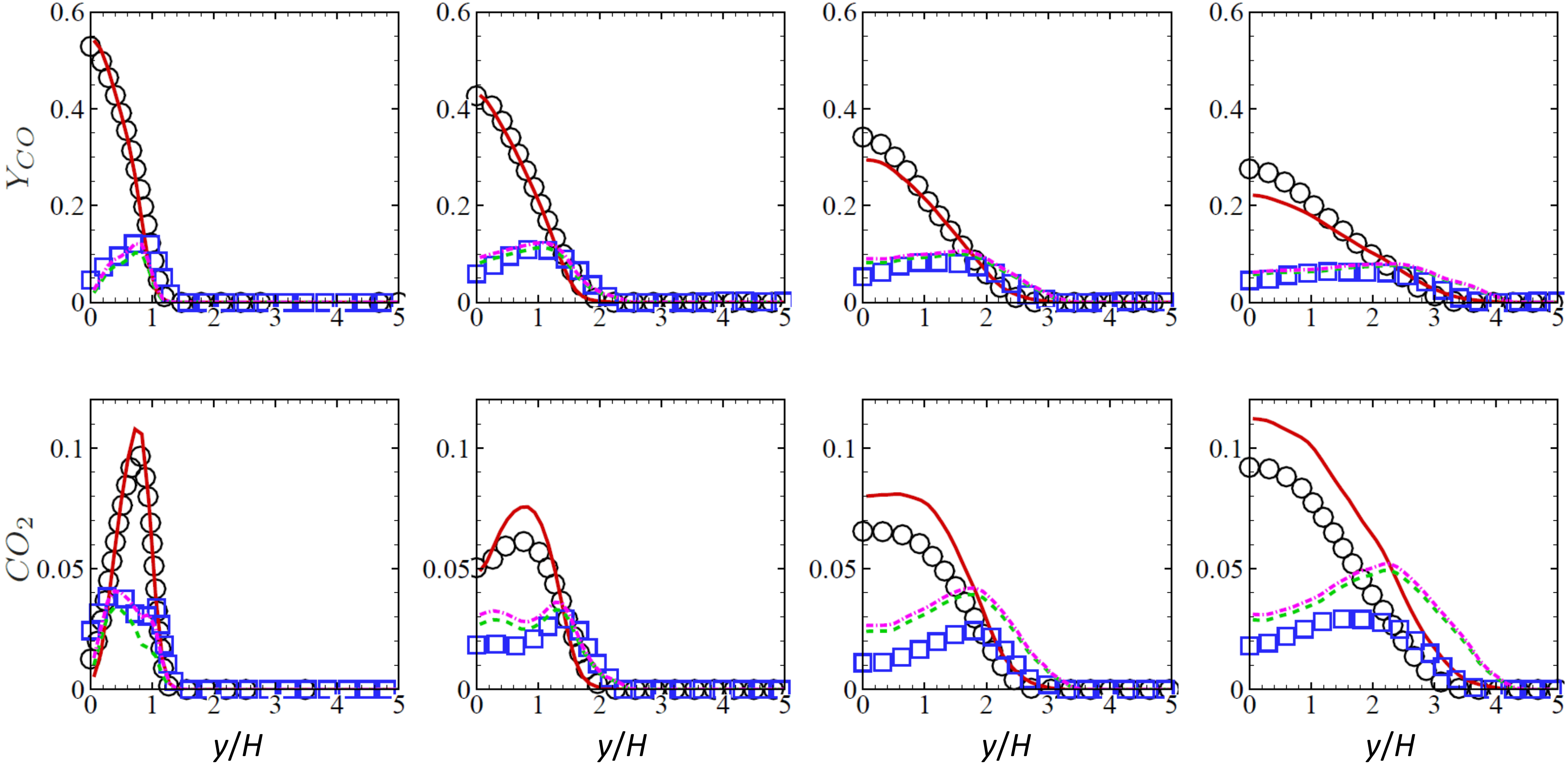
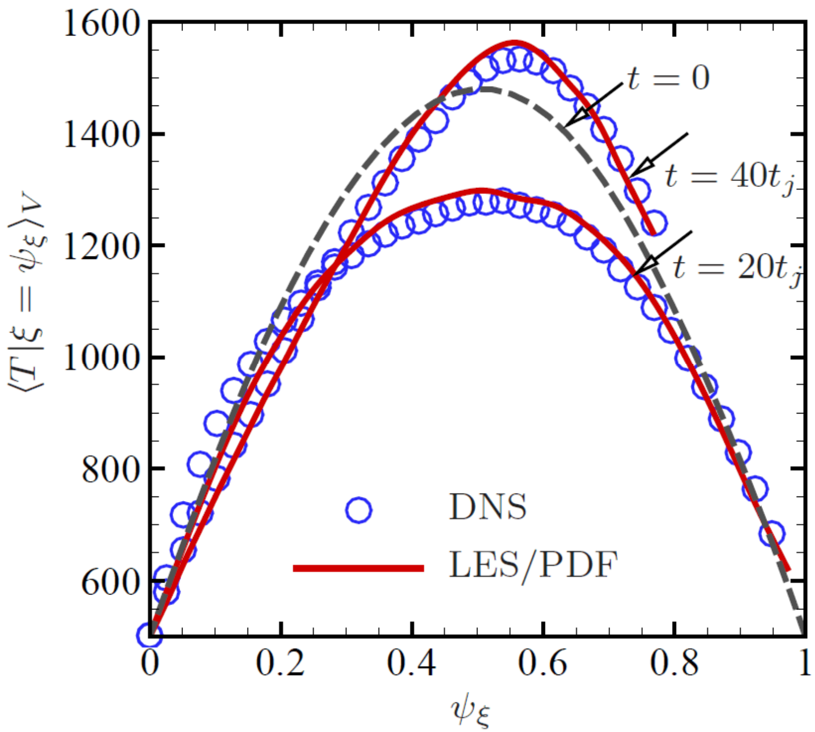


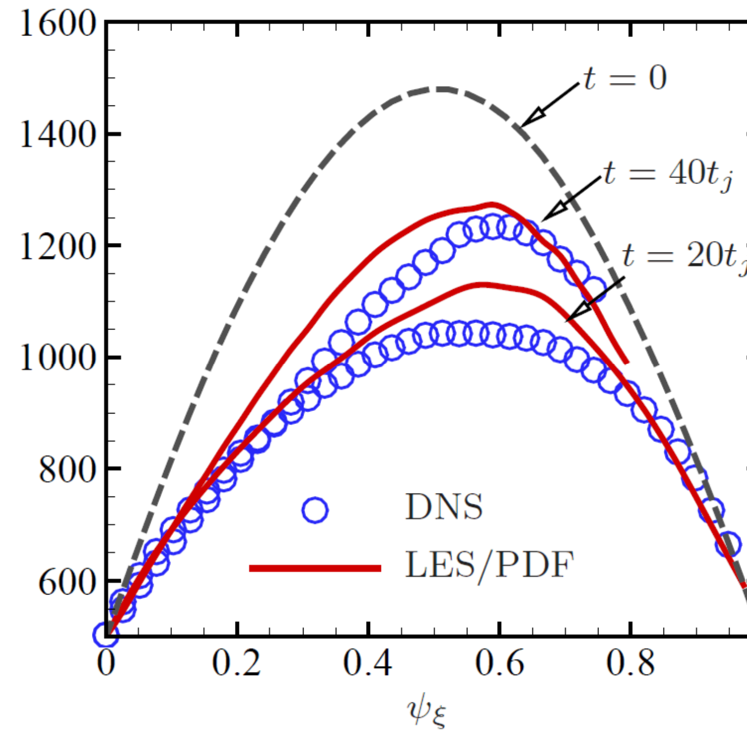
t = 10t_j *t* = 20t_j *t* = 30t_j *t* = 40t_j

Comparisons between DNS and LES/PDF: Conditional mean temperature

- Good prediction of local extinction and re-ignition in LES/PDF



Re = 2510



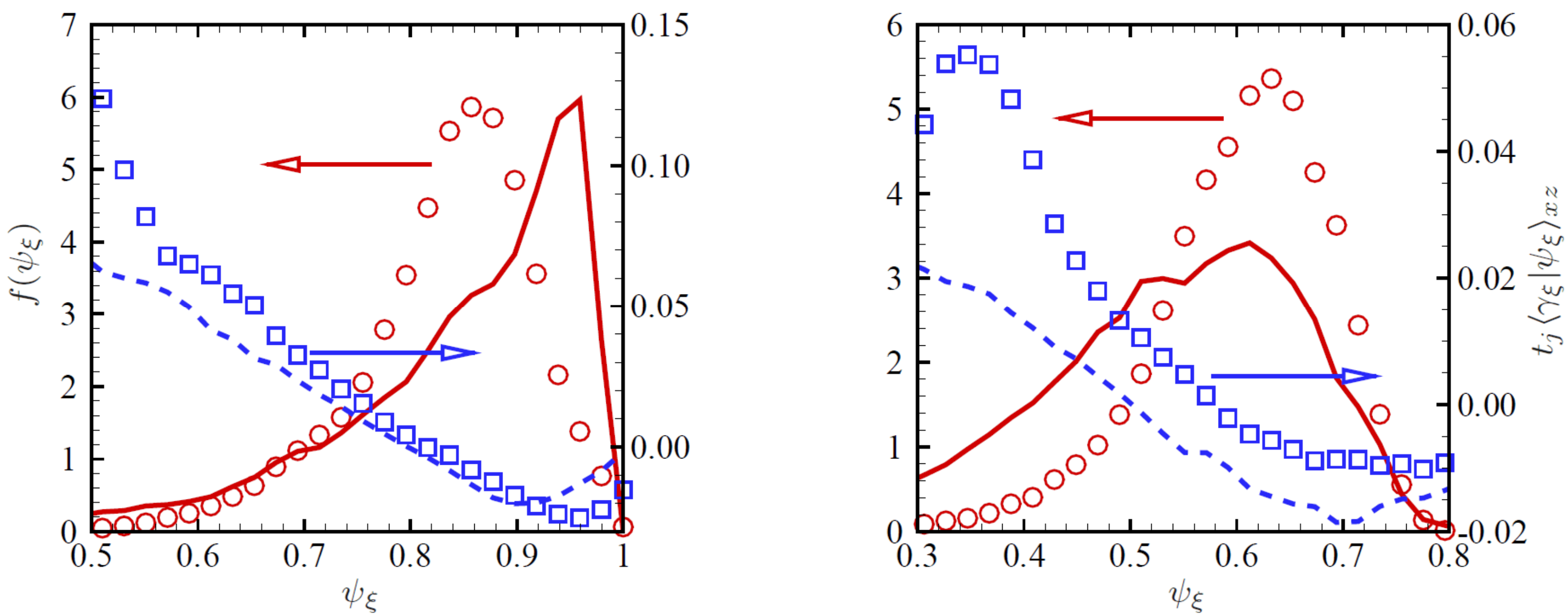
Re = 9079

Conditional diffusions of mixture fraction

- Underprediction of conditional diffusion $\gamma_\alpha(\boldsymbol{\psi}, \boldsymbol{x}, t) = -\Omega_m(\psi_\alpha - \widetilde{\phi}_\alpha) + \widetilde{\mathcal{D}}$
- Cause the slower relaxation of the PDF and the slight underprediction of the mean mixture fraction

PDFs of mixture fraction ○: DNS ——: LES/PDF

Normalized conditional diffusion □: DNS ---: LES/PDF



$t = 20t_j$ $t = 40t_j$

Normalized conditional diffusion and PDFs of mixture fraction at $y/H = 0$

Modeling of multi-scalar mixing in LES/PDF

- Modeling of scalar mixing is crucial in the PDF method
- Most mixing models use only scalar-space variables and do not take into account the spatial scalar structure

- Previous studies of the multi-scalar mixing in nonreacting flows
- Lack of *a priori* and *a posteriori* tests of the PDF modeling of multi-scalar mixing in turbulent reacting flows
- Mixing term in the PDF transport equation can be exactly obtained from DNS
- Comparisons between DNS and LES/PDF

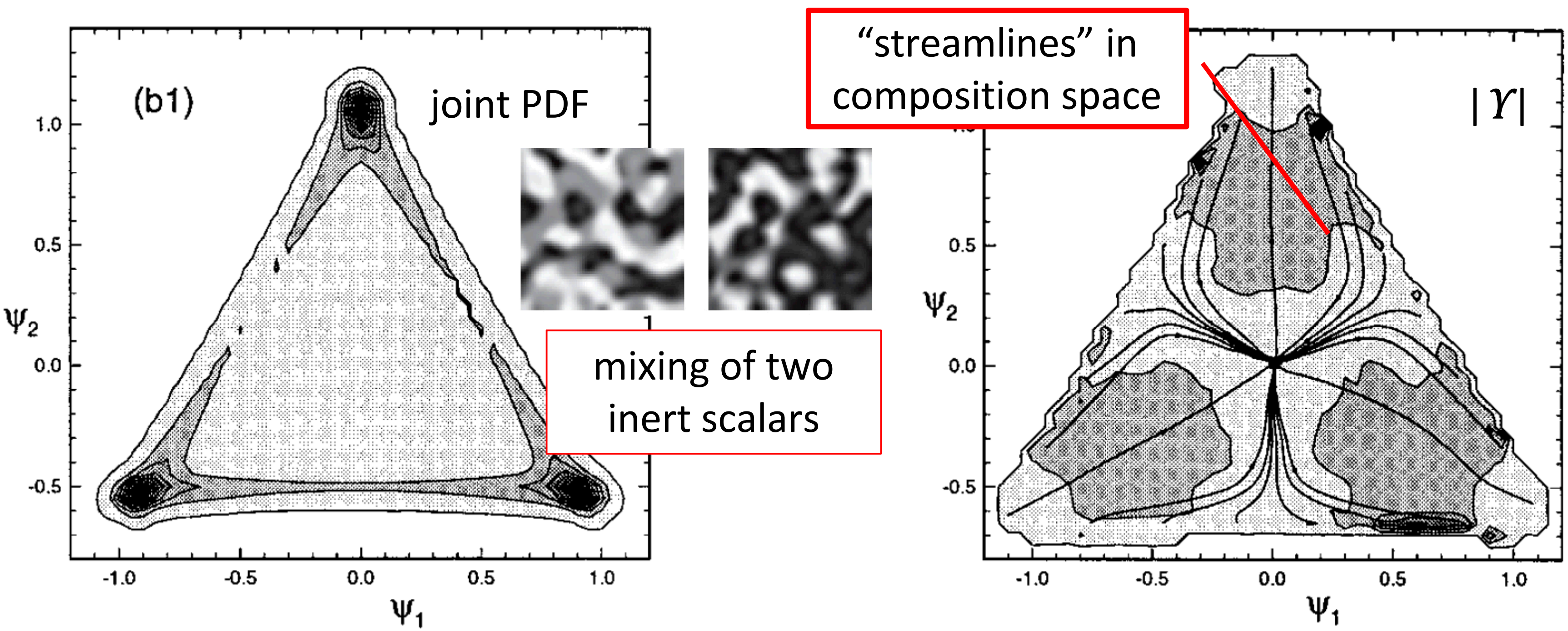
Multi-scalar mixing in isotropic nonreacting turbulence

- One-point, one-time joint PDF $f = f(\boldsymbol{\psi}; \boldsymbol{x}, t)$

$$\frac{\partial f}{\partial t} + \nabla \cdot [f(\langle \boldsymbol{U} \rangle + \langle \boldsymbol{u} | \boldsymbol{\psi} \rangle)] = -\frac{\partial}{\partial \psi_\alpha}[f(\langle \Gamma_{(\alpha)} \nabla^2 \phi_\alpha | \boldsymbol{\psi} \rangle + S_\alpha(\boldsymbol{\psi}))]$$

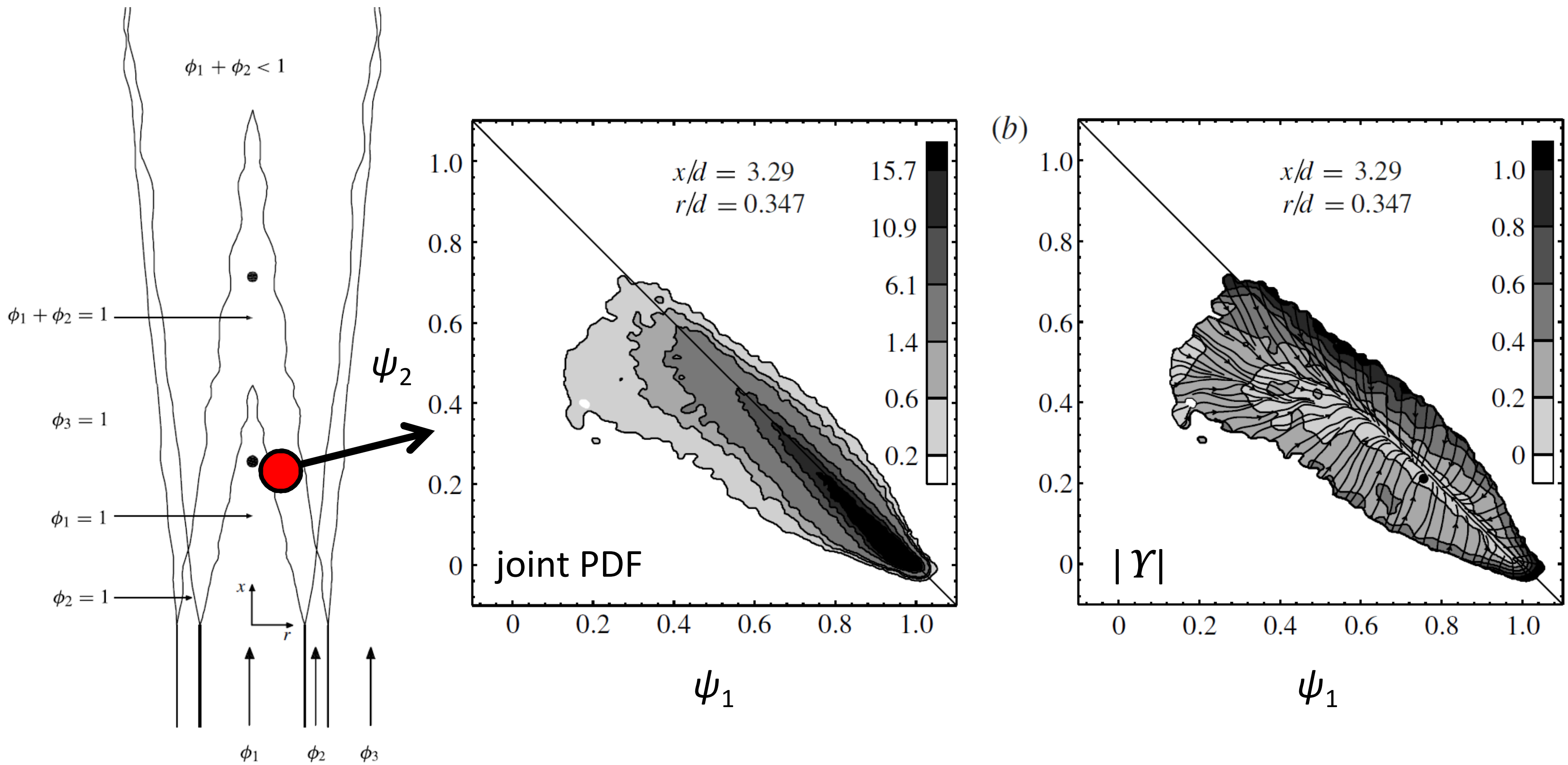
- “Velocity” in composition space

$$\gamma_\alpha(\boldsymbol{\psi}, t) = \langle \Gamma_{(\alpha)} \nabla^2 \phi_\alpha | \boldsymbol{\psi} \rangle = -\Omega_m(\psi_\alpha - \langle \phi_\alpha \rangle)$$



A. Juneja and S. B. Pope, *Phys. Fluids* (1996)

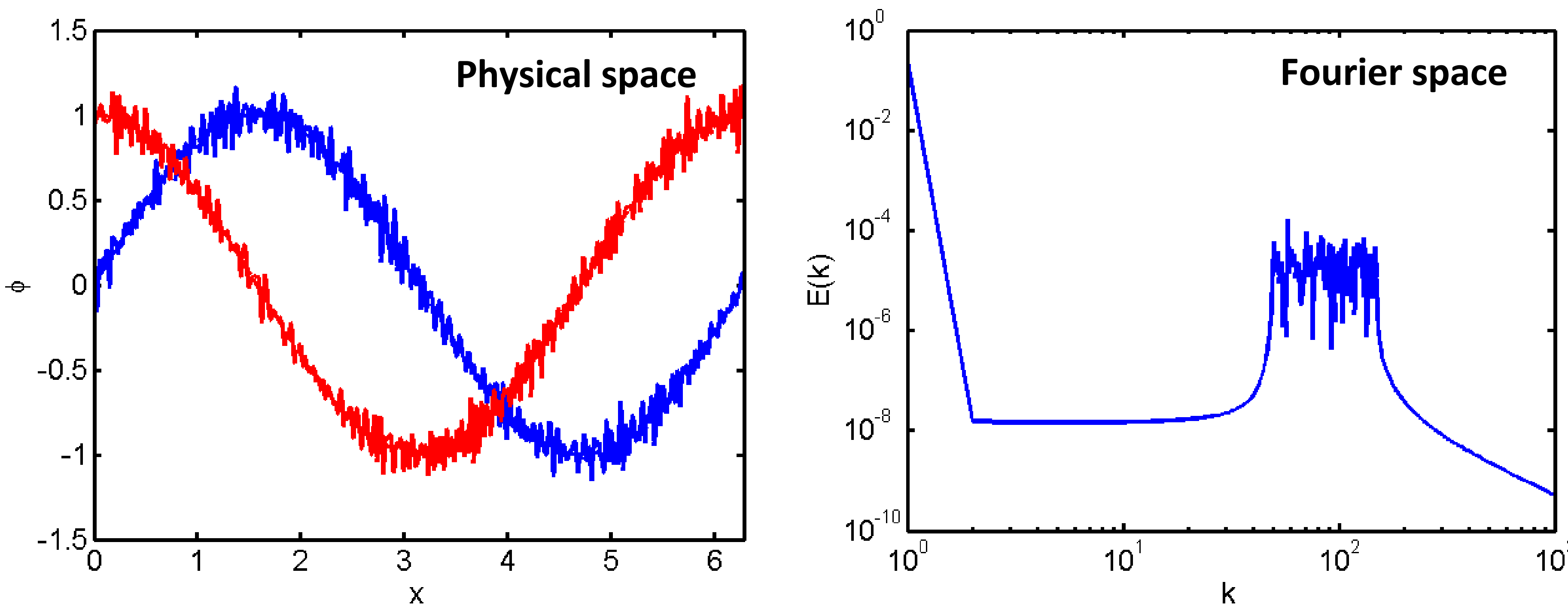
Multi-scalar mixing in nonreacting coaxial turbulent jet



- Mixing of the two scalars can occur only through the third, forcing a detour of the manifold in scalar space

J. Cai et al., *J. Fluid Mech*. (2011)

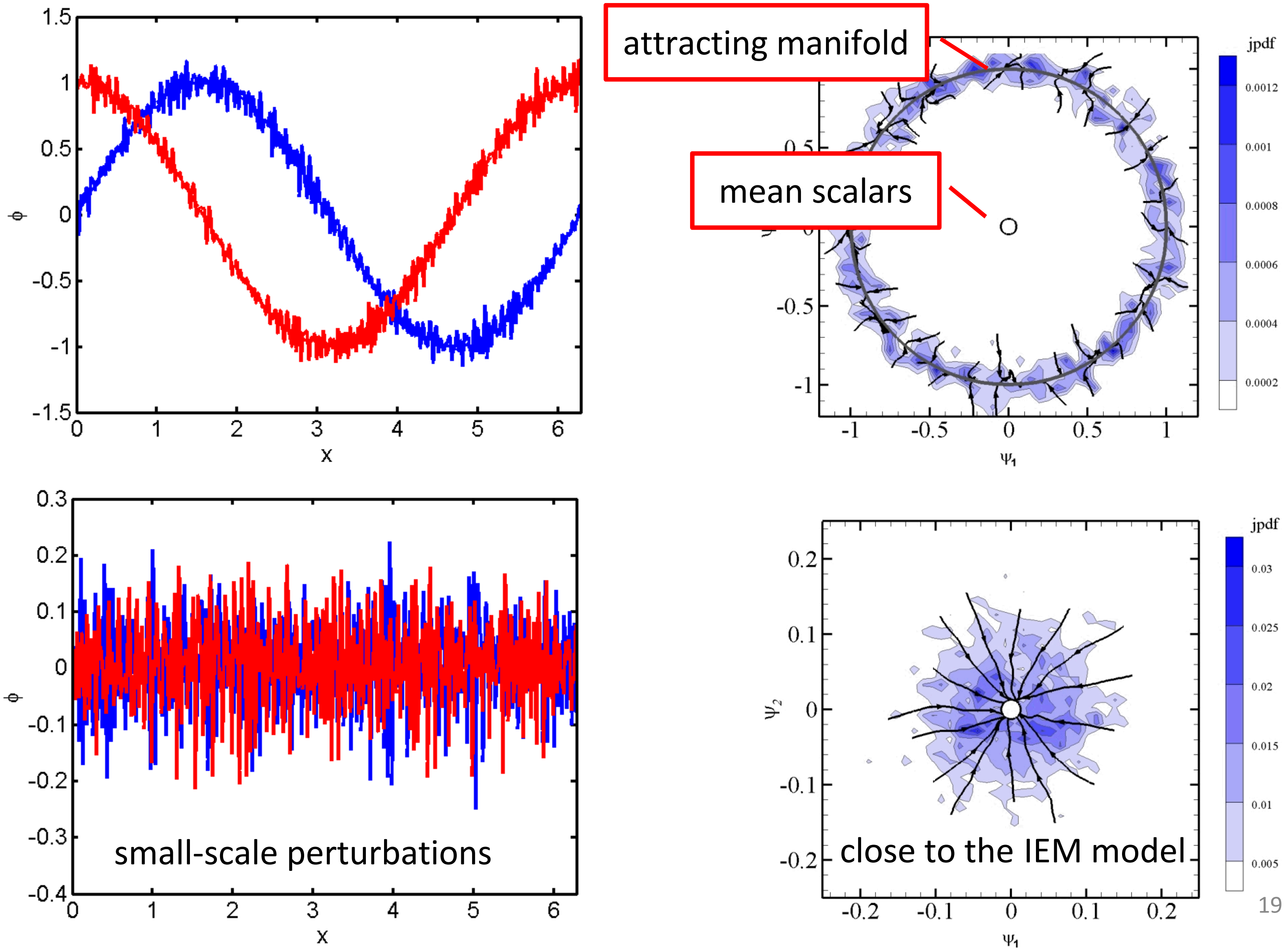
Example of the mixing of two 1D scalars



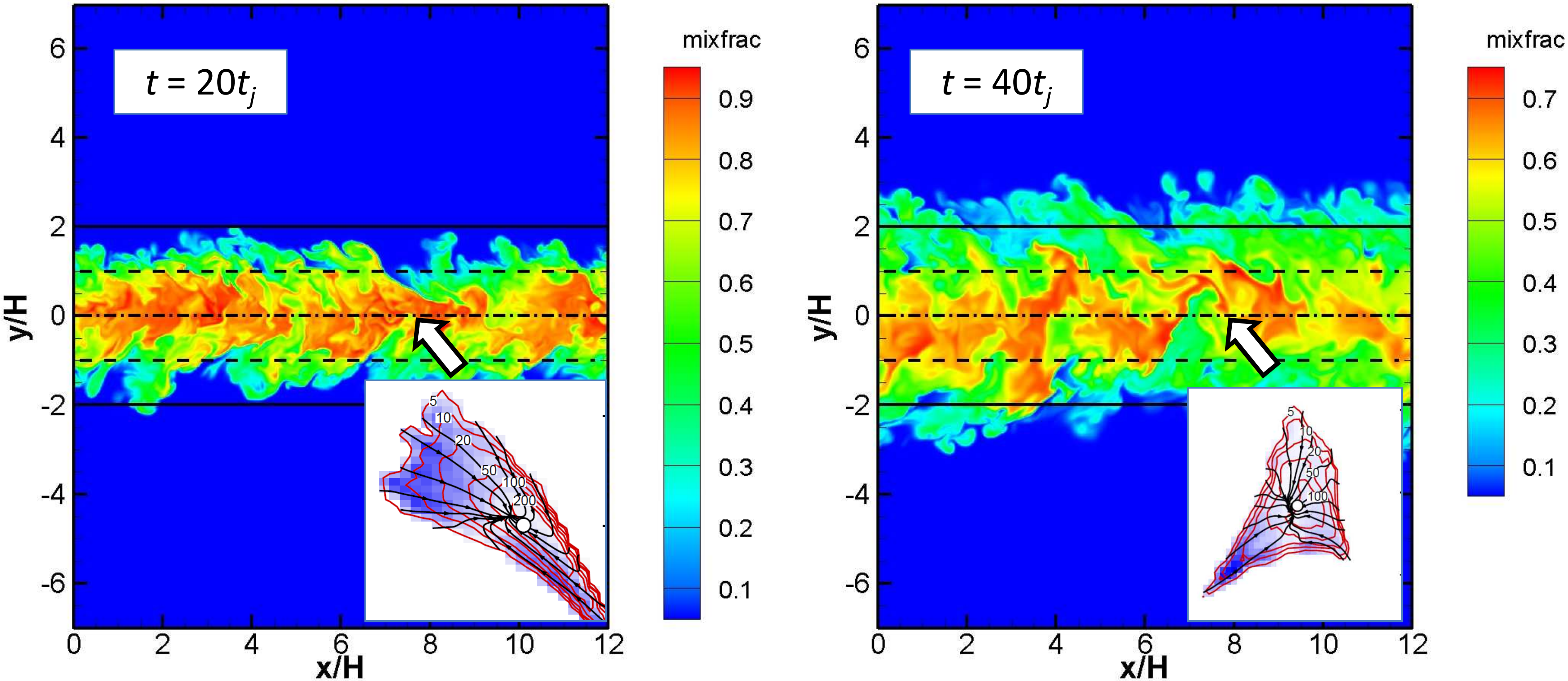
- 1D scalar function φ = a large-scale function + small-scale fluctuations
- = **sin(*x*)** or **cos(*x*)** +

  random Fourier modes at high wavenumbers
- $\phi_0 = \sin(kx)$, $d^2\phi_0/dx^2 = -k^2\sin(kx) = -k^2\phi_0$

Mixing of two 1D scalars in the domain [0,2π]



Multi-scalar mixing in composition space at different stages



Contours of the mixture fraction on the *x*-*y* plane

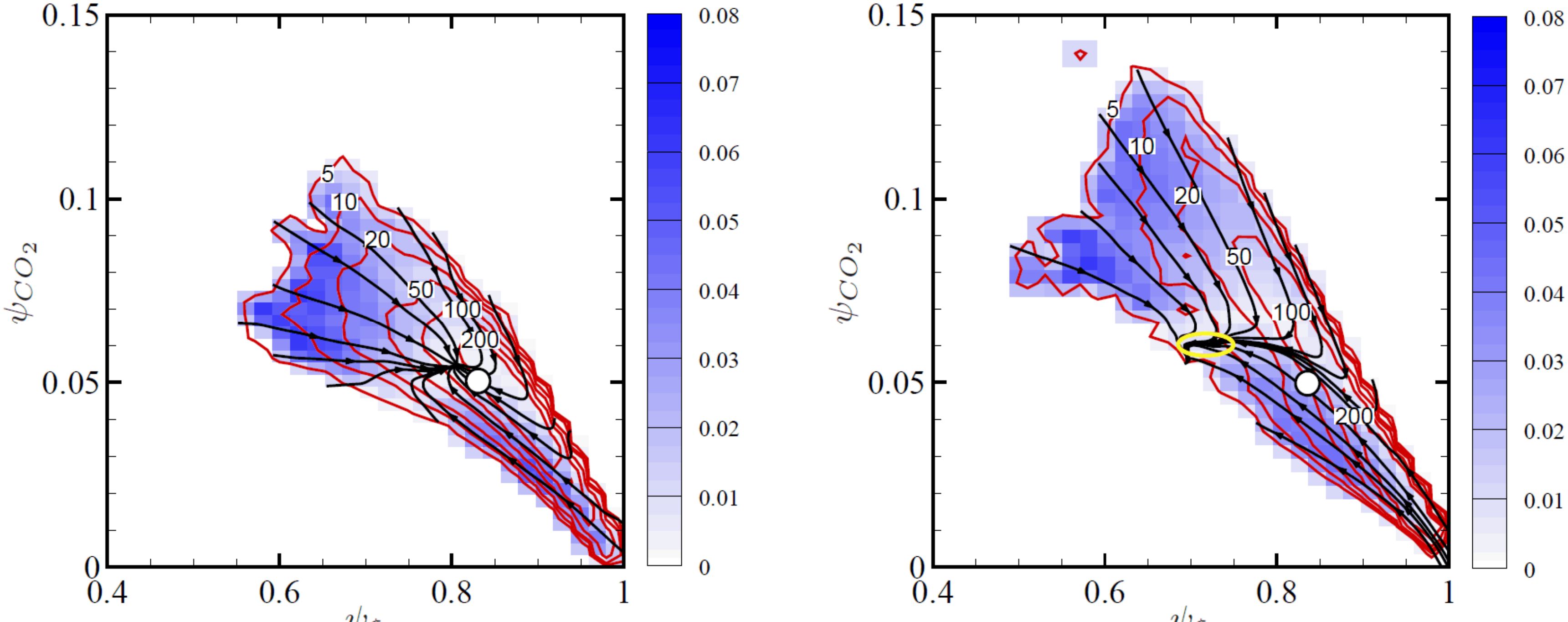
- Joint PDFs of the mixture fraction and Y_{CO2} (a progress variable) on the *x*-*z* plane
- Manifold in composition space near the shear layer or at the early stage (transition from laminar flow to turbulent flow)
- Close to the IEM model in the fully developed turbulent region

Multi-scalar mixing in composition space (t = 20t_j, y/H=0)

- Approximation of the attracting manifold $\mathcal{M}(\psi) \equiv \|\psi - \widehat{\phi}(\psi)\|_2 = 0$
- RANS/PDF: $\widehat{\phi}_\alpha = \langle \phi^*_\alpha \rangle_{xz}$ LES/PDF: $\widehat{\phi}_\alpha \approx \langle \langle \widetilde{\phi}^*_\alpha | \psi \rangle \rangle_{xz}$

—— : joint PDF $f(\psi_\xi, \psi_{CO2})$ ▭ : normalized conditional mean diffusion velocity magnitude

○ : mean scalars ⬭ : approximation of the manifold in LES/PDF $M(\psi_\xi, \psi_{CO2}) \approx 0$



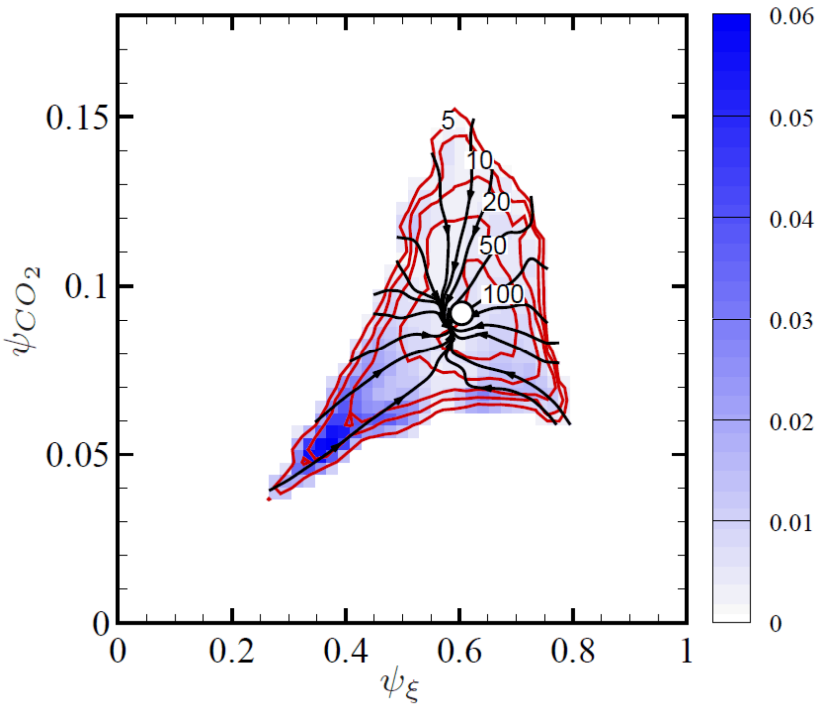
DNS LES/PDF

Multi-scalar mixing in composition space (t = 40t_j, y/H=0)

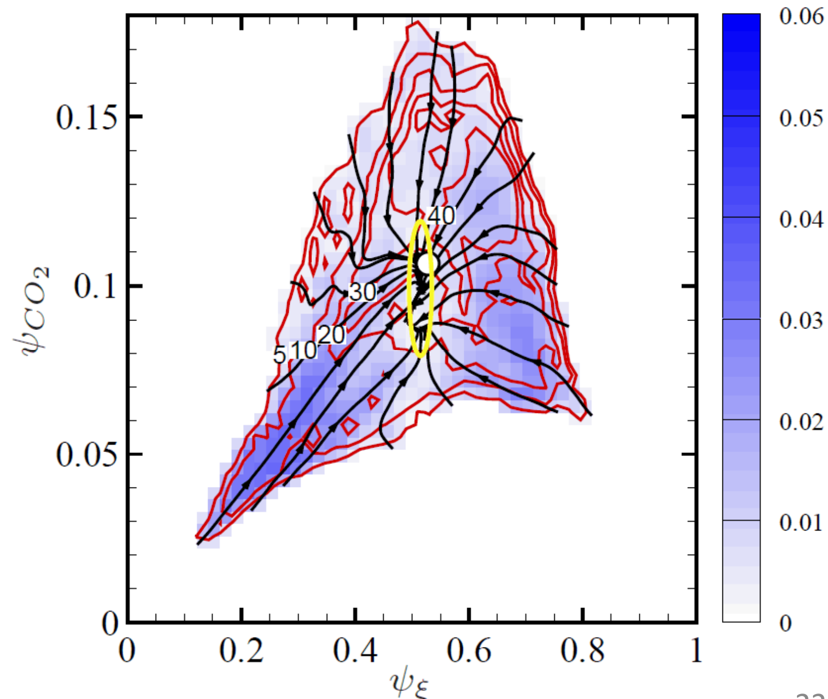
- Approximation of the attracting manifold $\mathcal{M}(\psi) \equiv \|\psi - \widehat{\phi}(\psi)\|_2 = 0$
- RANS/PDF: $\widehat{\phi}_\alpha = \langle \phi_\alpha^* \rangle_{xz}$ LES/PDF: $\widehat{\phi}_\alpha \approx \langle \langle \widetilde{\phi}_\alpha^* | \psi \rangle \rangle_{xz}$

— (red line): joint PDF $f(\psi_\xi, \psi_{CO2})$; (blue shading): normalized conditional mean diffusion velocity magnitude

○ : mean scalars; (yellow ellipse): approximation of the manifold in LES/PDF $M(\psi_\xi, \psi_{CO2}) \approx 0$



DNS



LES/PDF

Conclusions

- An accurate and scalable LES/PDF tool (NGA/HPDF code) for massive computational studies has been implemented
- Comparisons of DNS and LES/PDF for the non-premixed jet flame
  - Number of grid points in LES/PDF is less than 1/500 of the DNS
  - Good agreement of major quantities in low and high *Re* cases
  - Good prediction of local extinction and re-ignition
- Multi-scalar mixing in DNS and LES/PDF
  - DNS exhibits the attracting manifold at the early stage
  - LES/PDF shows qualitative agreement for the manifold and joint PDFs

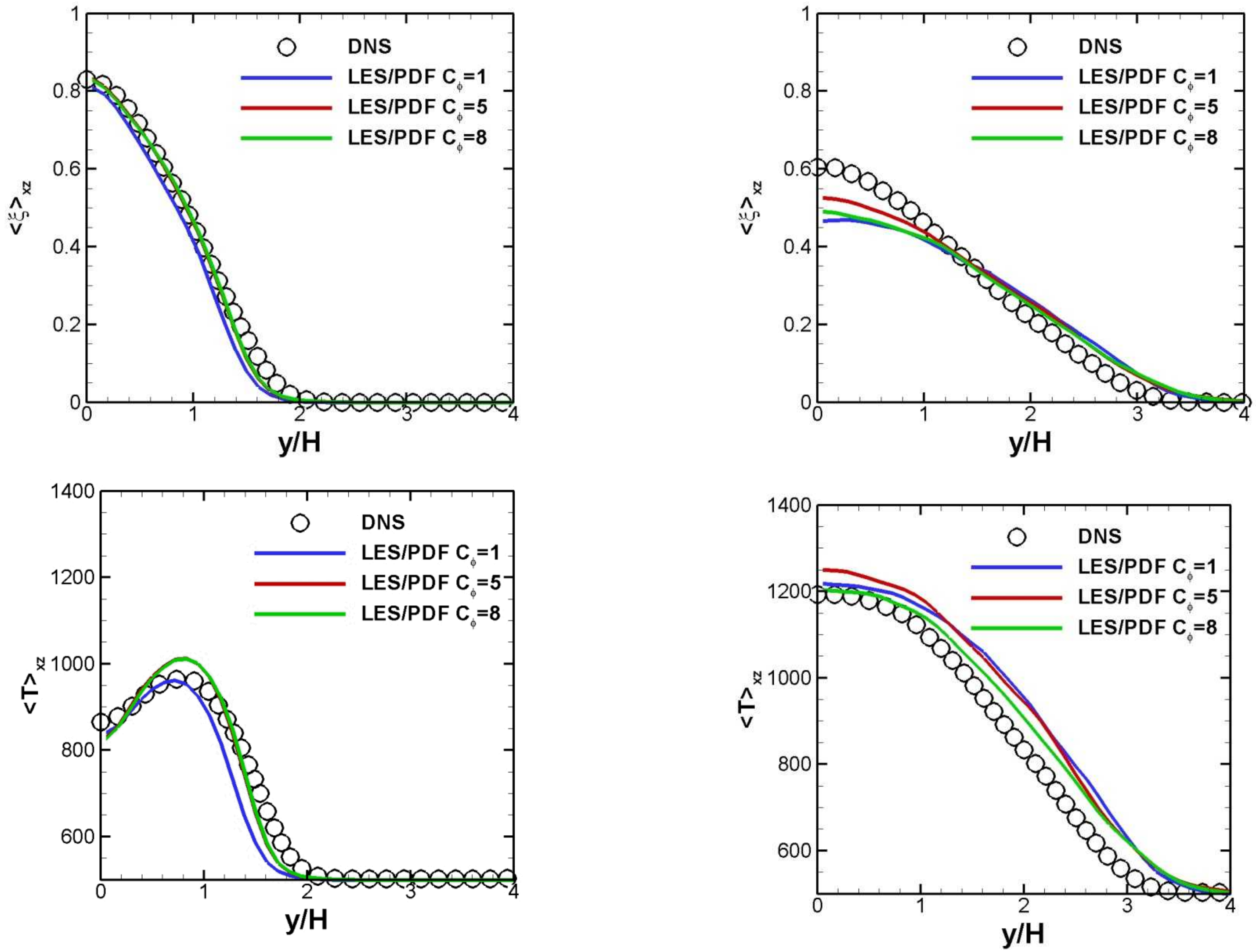
Acknowledgments

- This work is supported in part by the *Combustion Energy Frontier Research Center* (CEFRC) funded by the DOE
- E. R. Hawkes, H. Kolla, O. Desjardins, P. P. Popov

Thanks!

Please contact **Yue Yang** (yy463@cornell.edu) for further discussions.

Sensitivity of the model constant C_ϕ



Sensitivity of the filter width