

Turbulent Flame Structure of Cavity Stabilized Reacting Shear Layers: Effects of Flow Compressibility, Heat Release, and Finite-rate Kinetics

Harsha Chelliah, Chris Goyne, Bob Rockwell

University of Virginia

Jack Edwards

NC State University

Andrew Cutler

George Washington University

Paul Danehy

NASA Langley Research Center

Jackie Chen

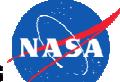
SANDIA Livermore

AFSOR-ARO-NSF Basic Combustion Research Review

August 28-30, 2018, Arlington, VA



Sandia
National
Laboratories



NC STATE UNIVERSITY

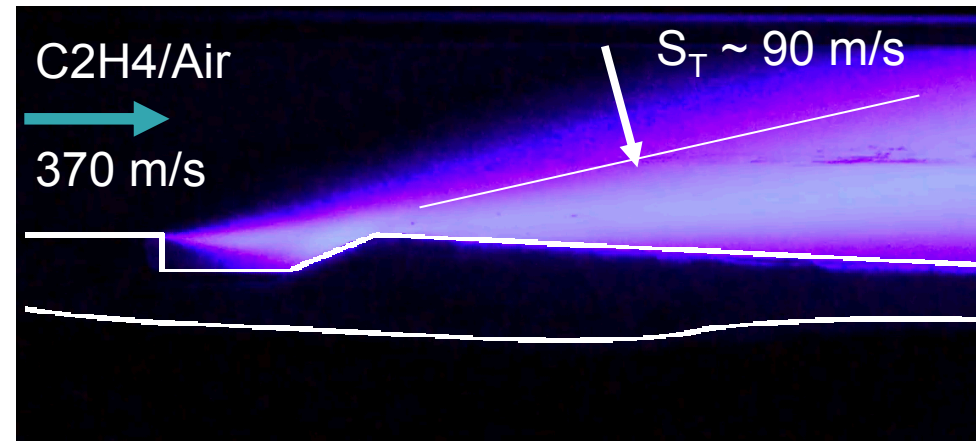


Objectives/Background

□ Cavity stabilized flames

provide a **canonical** configuration to study:

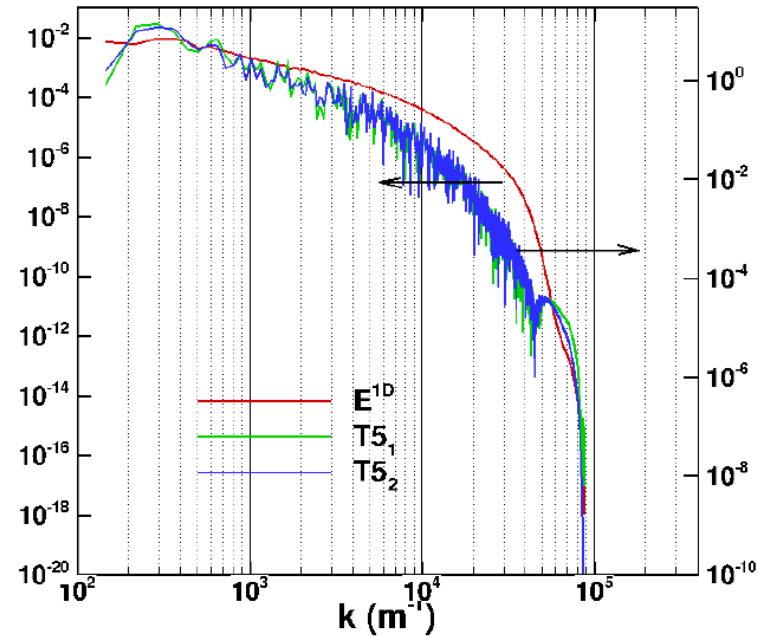
- compressible, premixed, turbulent flames (M_c , ϕ , u') with a significant flame normal velocity component
- Extraction of turbulent spectra [$E(k)$ vs. k] or flame structure [Re vs Da] information with high-resolution diagnostics, LES, and DNS
 - eg. OH-PLIF maximum resolution of $39 \times 39 \times 25 \mu m$



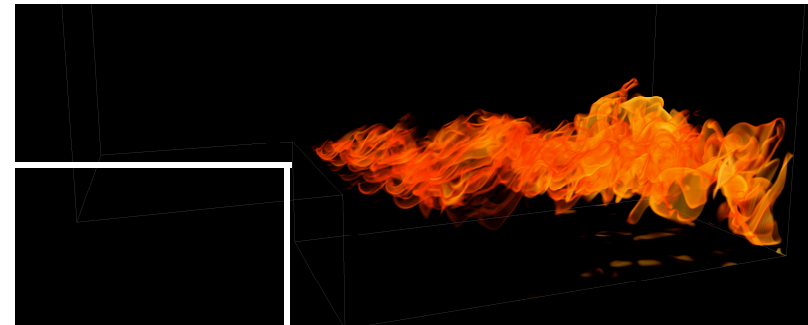
□ Provide a comprehensive database for turbulence model development/validation under Air Force relevant conditions

Objectives/Background (cont.)

- ❑ In compressible flows, **pressure-velocity correlations (T5 in fig)** can account for a significant fraction of TKE at high wave numbers (Kolla et al., 2013)
- ❑ Similar findings by DNS work by Sarkar and co-workers, including effects of convective Mach number
- ❑ Since high wave numbers cannot be resolved by experiments and LES, **DNS is the only option!**

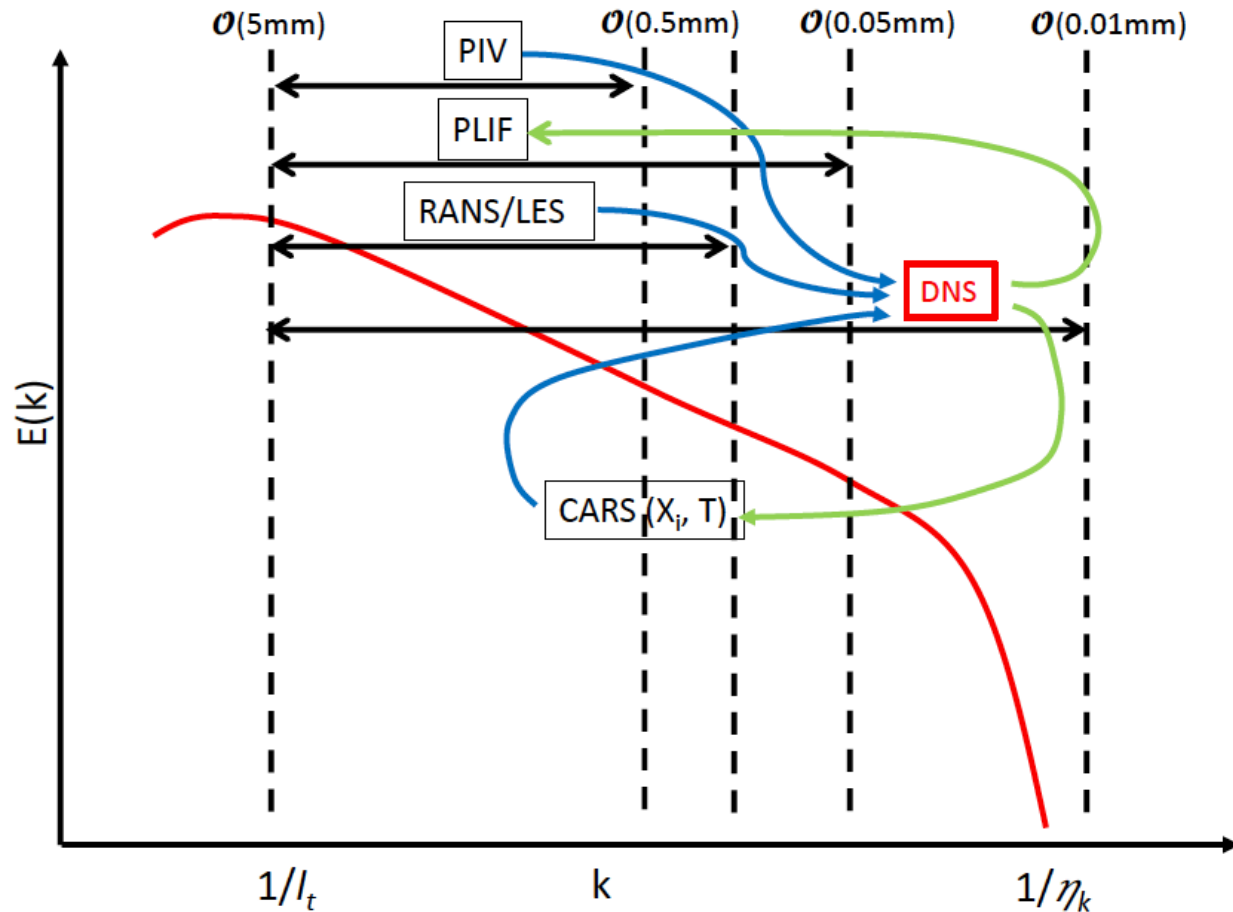


Spectra from preheated H₂/air premixed turbulent flame (Kolla et al. JFM 2013).



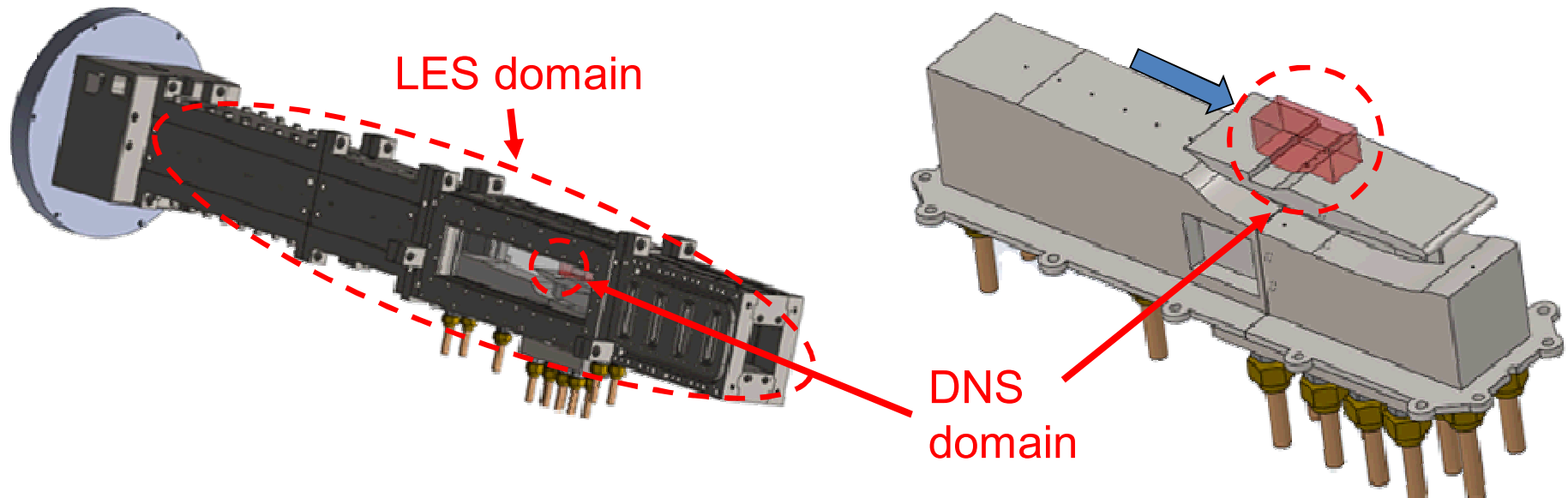
Heat release rate in a backward facing step (Konduri, Chen et al.)

Our Approach – A Hybrid Method



- For varying heat release and flow compressibility, investigate the premixed, turbulent flame structure/ statistics via DNS, RANS/LES, PIV, PLIF, CARS.

Flow Path and Computational Domains



- For the DNS domain, with a viscous length scale $\delta_v = 2.5 \mu\text{m}$ and 1/3 scale cavity (H=3 mm, L=18 mm) → 15 B grid points
- Estimated 3D computational cost: **75 million CPU hours!!!**
- In RANS/LES, 90 M grid points with a resolution of about $300\mu\text{m}$

DNS of cavity stabilized premixed turbulent flame with a high-order immersed boundary method
A.H. Rauch, K. Aditya, H. Kolla, J.H. Chen, H.K. Chelliah

Parametric Conditions Explored

Test matrix:

	High heat release (ER $\approx$ 0.46)	Low heat release (ER $\approx$ 0.36)	No heat release
High Mach # (M $\approx$ 0.7)		Case 2	
Low Mach # (M $\approx$ 0.63)	Case 1	Case 3	Case 4

- Third parameter, turbulent intensity (u'/U) variation efforts are on-going!

Key Non-dimensional Parameters

Conditions at highest ER:

$$\phi_{global} = 0.48; \quad \phi_{local} = 0.6; \quad S_L = 6 \text{ m/s}$$

$$\overline{u_x} = 370 \text{ m/s}; \quad M \approx 0.63$$

$$u'_1 = 45 \text{ m/s}; \quad u'_2 = 30 \text{ m/s}$$

$$(l_t)_{11} \approx 12 \text{ mm}; \quad (l_t)_{22} \approx 4 \text{ mm}$$

$$(Re_t)_{11} = \frac{u'_1 l_t}{\nu} \approx 4100; \quad (Re_t)_{22} \approx 950$$

- Assuming constant energy dissipation rate and isotropic turbulence:

$$\eta_k = \frac{l_t}{Re_t^{3/4}} \approx 20 \text{ } \mu\text{m};$$

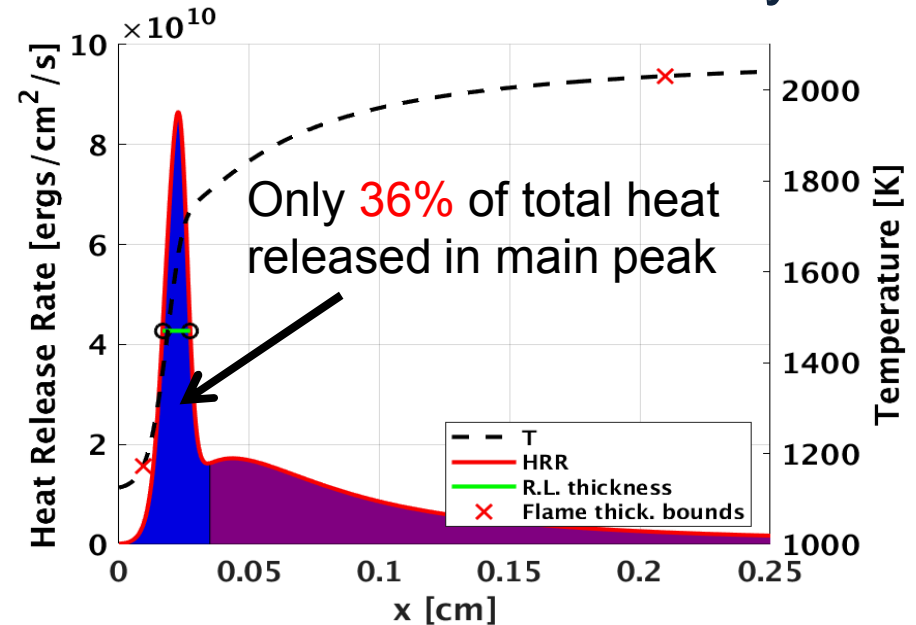
$$Ka = \frac{1}{Da_k} = \frac{\tau_c}{\tau_k} = \frac{\delta_f / S_L^0}{\eta_k / u'_k} \approx 10-120$$

Laminar Flame Thickness

- What is the flame thickness δ_f at conditions near the cavity?

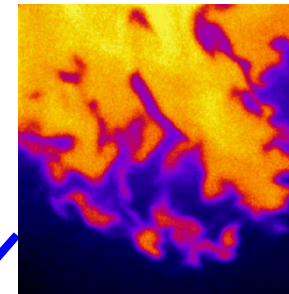
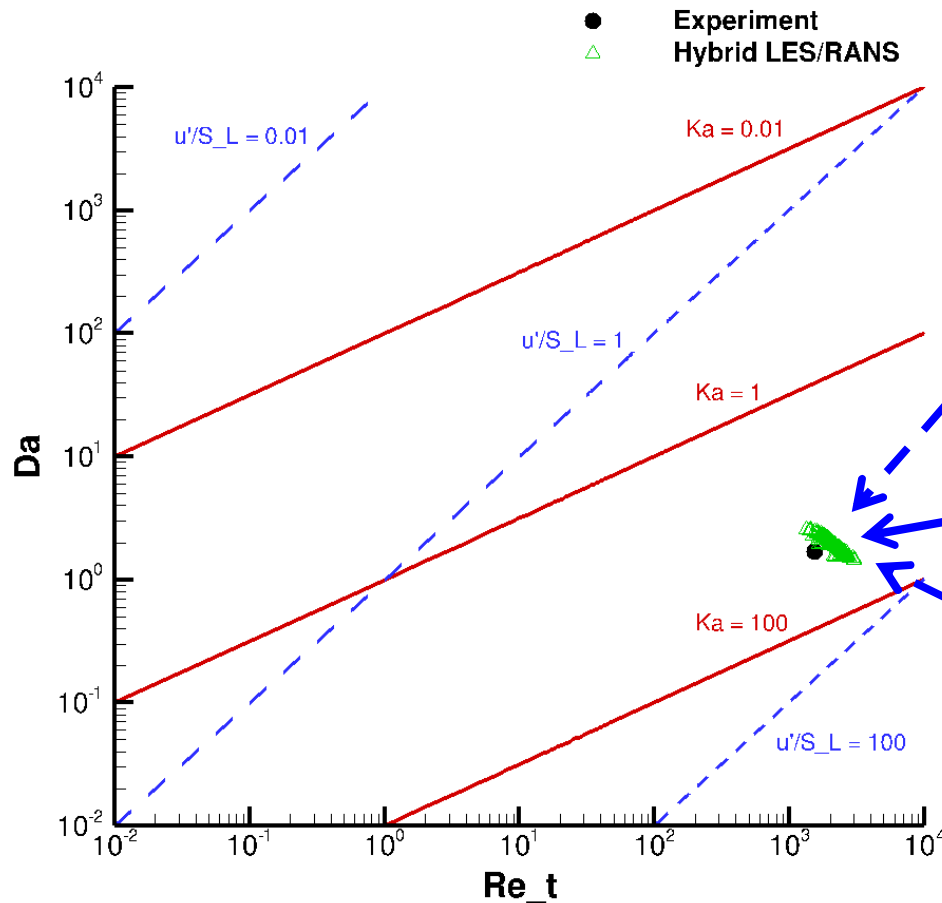
L (mm)	STP	$M_{\text{flight}} = 5$
$\delta_{\text{r.l.}}$	0.43	0.11
$\delta_{f,5\%}$	3.80	2.00
$\delta_{f,dT/dx}$	2.31	0.21

*unstretched flames without heat loss

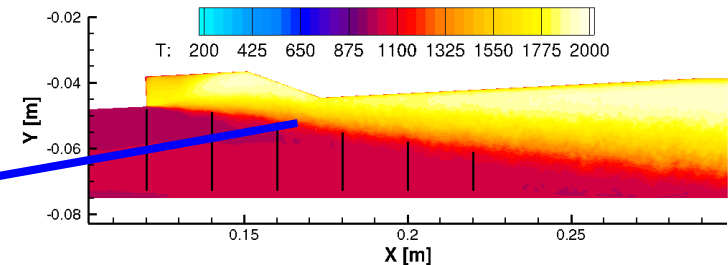


- Turbulent eddies can have a profound effect post-flame heat release region and S_T
- Key reactions contributing to post-flame heat release region are being analyzed

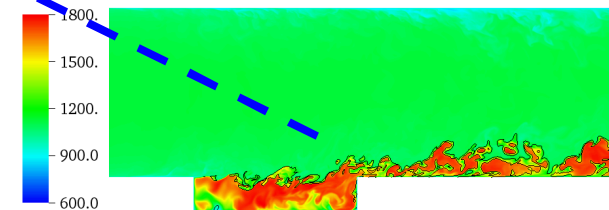
Re-Da Regime Diagram at M=0.6



From high-resolution PLIF



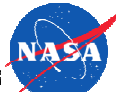
From hybrid RANS/LES



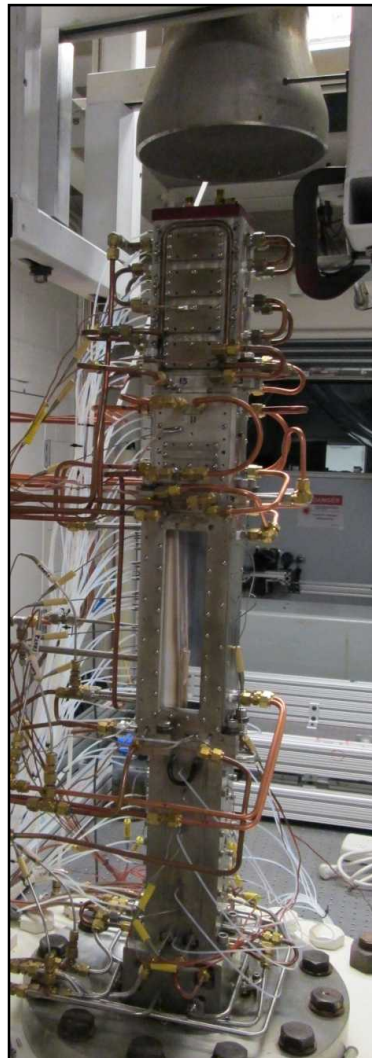
From DNS

Outline of Rest of the Presentation

- UVa high-enthalpy facility, new cavity insert
- Diagnostics (PIV, PLIF, CARS)
- Simulations (RANS/LES, DNS)



UVA Supersonic Combustion Facility



Extender

Combustor

Isolator

Nozzle

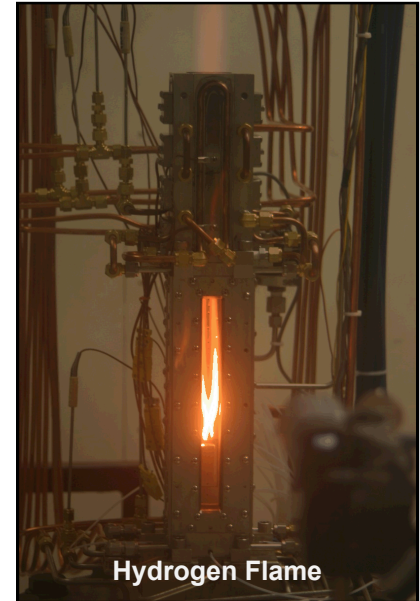
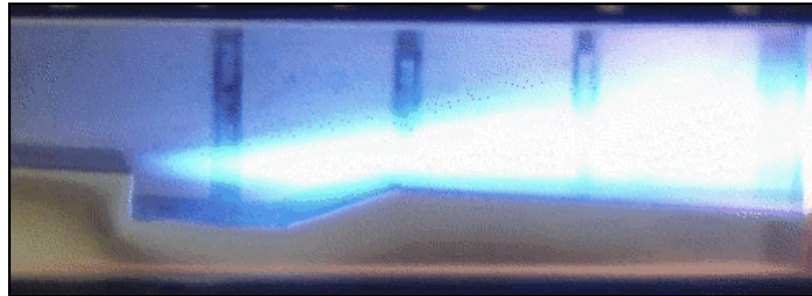
UVASCF Test Section

Facility:

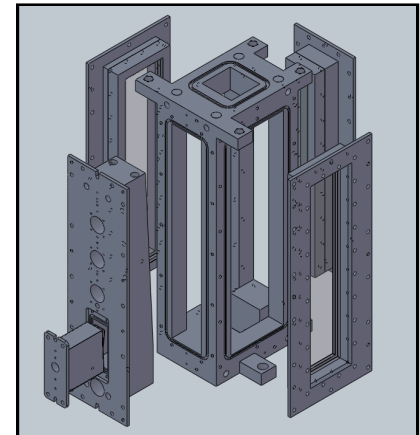
- Electrically heated, clean air flow to $T_0=1200$ K (simulated M5 flight enthalpy, 1.4 MJ/kg)
- **Continuous flow testing (6+ hours)**
- M2 or M3.2 facility nozzles
- Air flow of 0.2 kg/s ($p_0=300$ kPa)
- Hydrogen and ethylene fueling

Test Section:

- Dual mode scramjet with lineage to AFRL and NASA flow paths
- Modular hardware design
- Large quartz windows for imaging
- Slotted walls for CARS
- Independent combustor back pressuring via air throttle



Hydrogen Flame



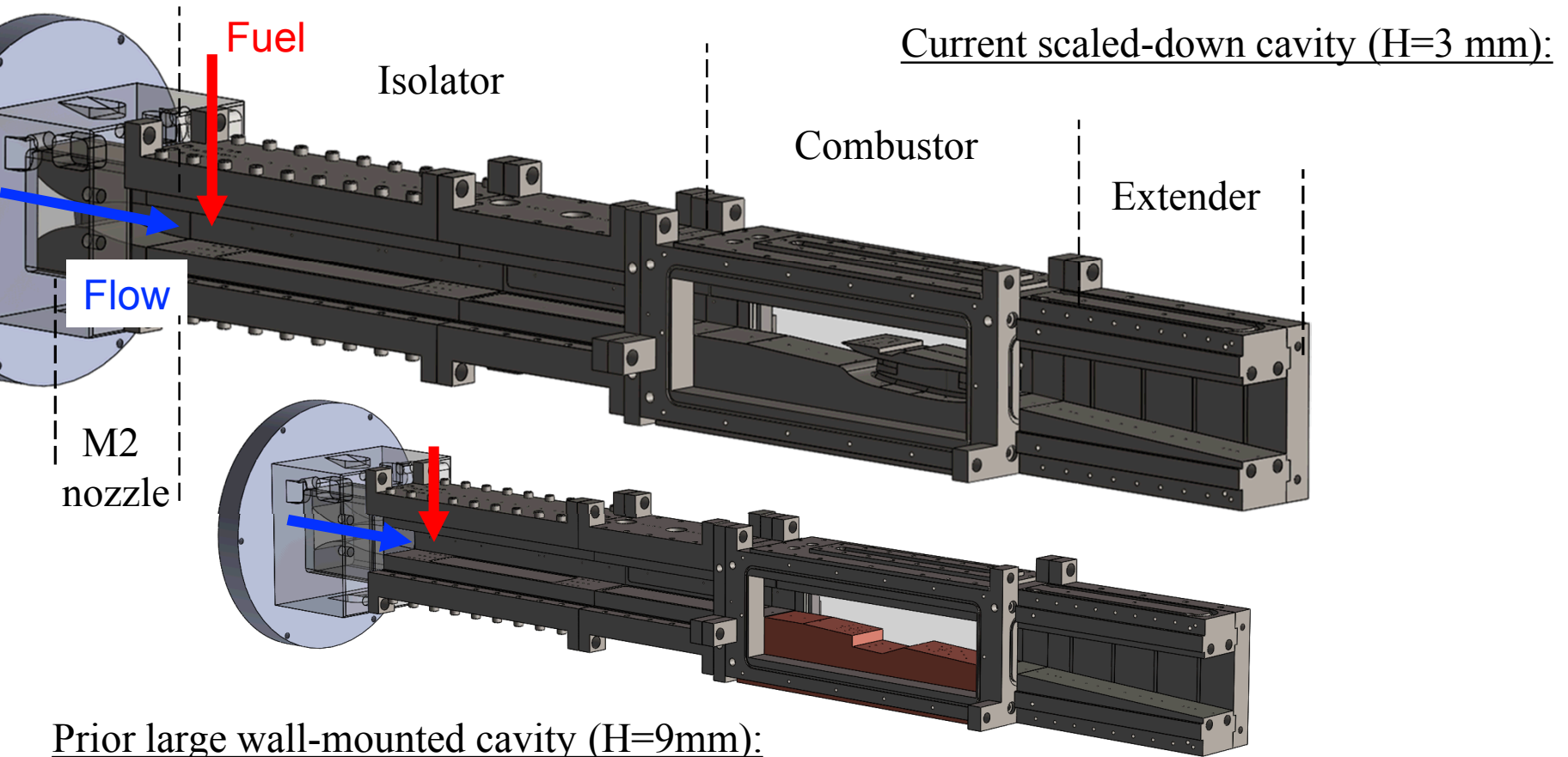
Modular Combustor



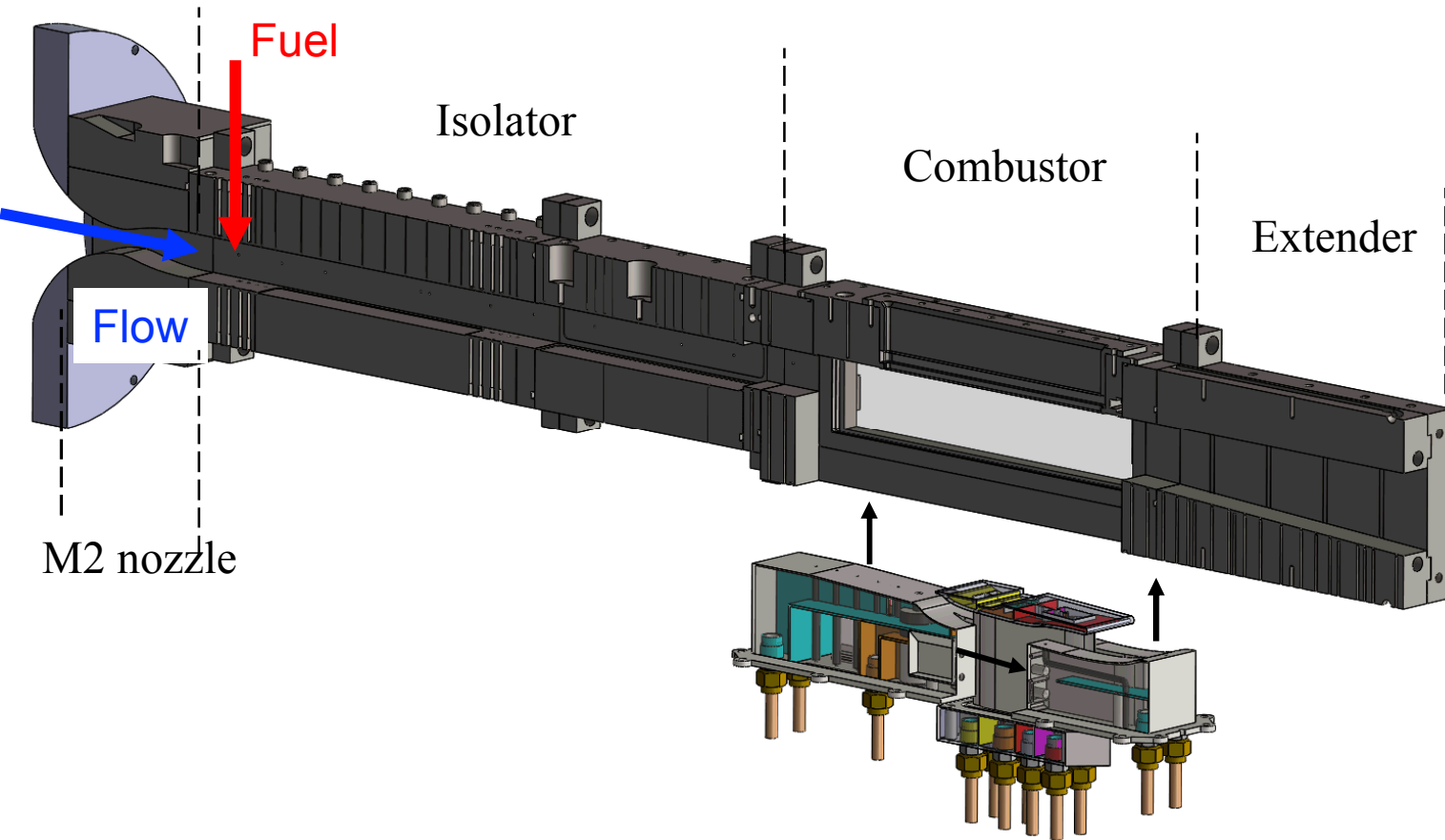
NC STATE UNIVERSITY



Large Wall-Mounted Cavity vs. Scaled-Down 3D Printed Cavity

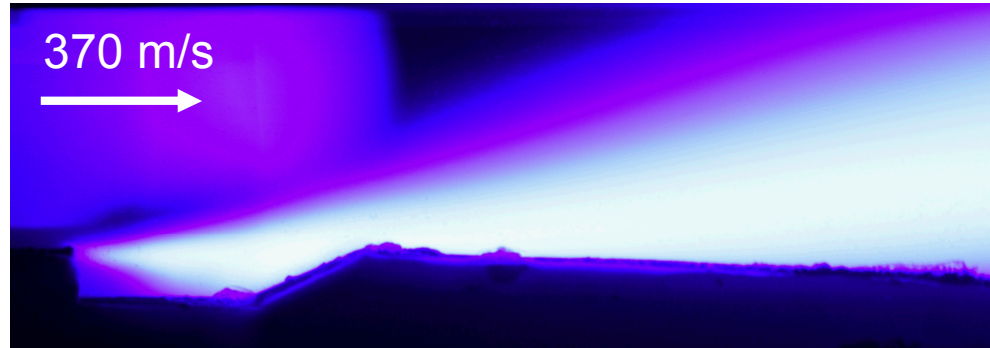


Modular Design

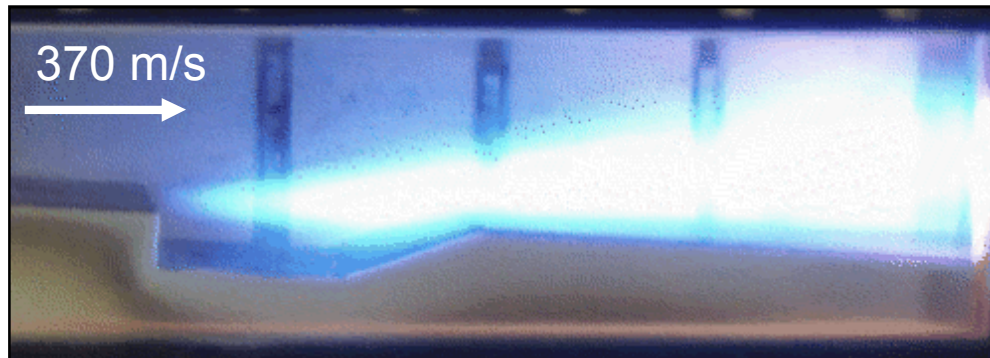


Comparison with Large Wall-Mounted Cavity

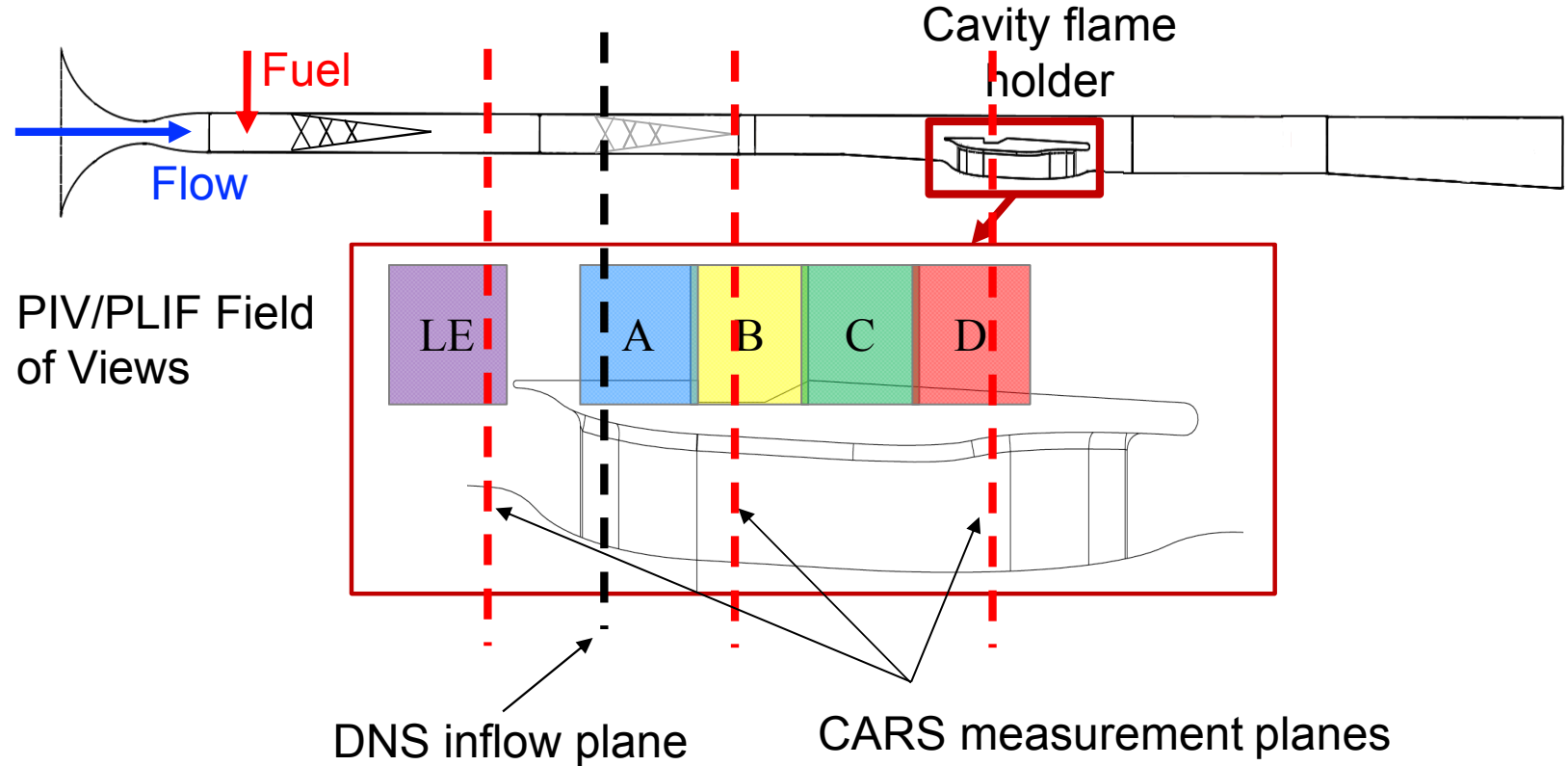
Strut mounted **1/3 scale cavity** [global $\Phi = 0.43$, local $\Phi \sim 0.55$, $M \sim 0.6$], $H=3\text{mm}$



Wall mounted **large cavity** [global $\Phi = 0.42$ (same as local), $M=0.6$], $H=9\text{mm}$



Experimental Measurement Planes, FOV's



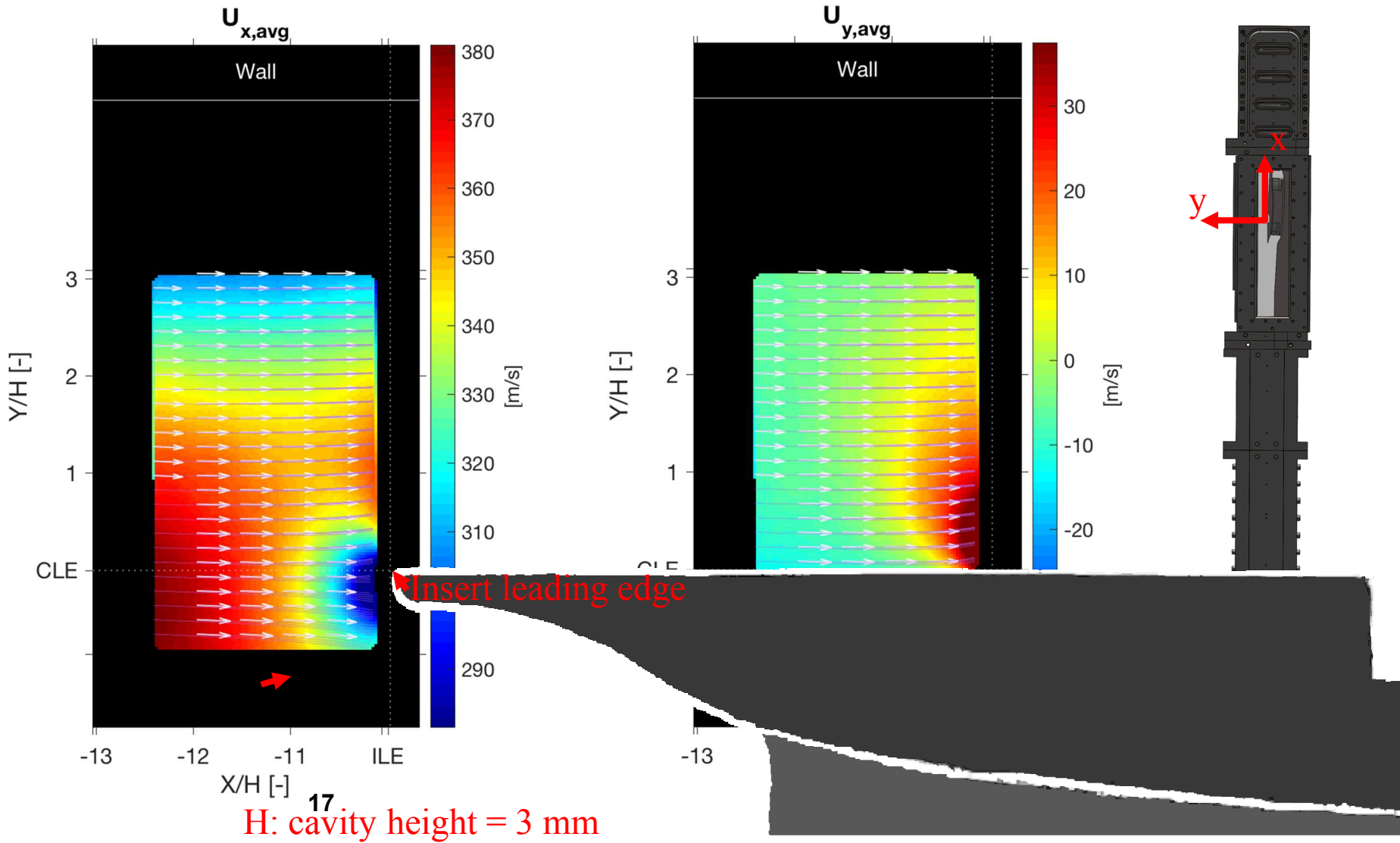
Diagnostics

- Velocity (2D mean, rms), integral length scales using PIV
- OH, CH₂O PLIF imaging
- Species and temperature using CARS



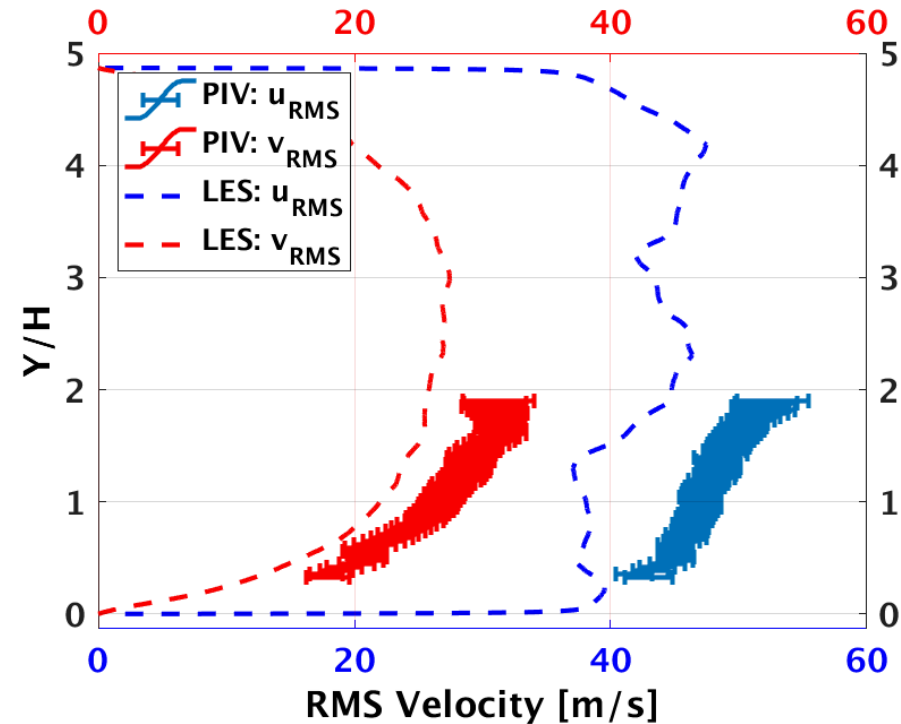
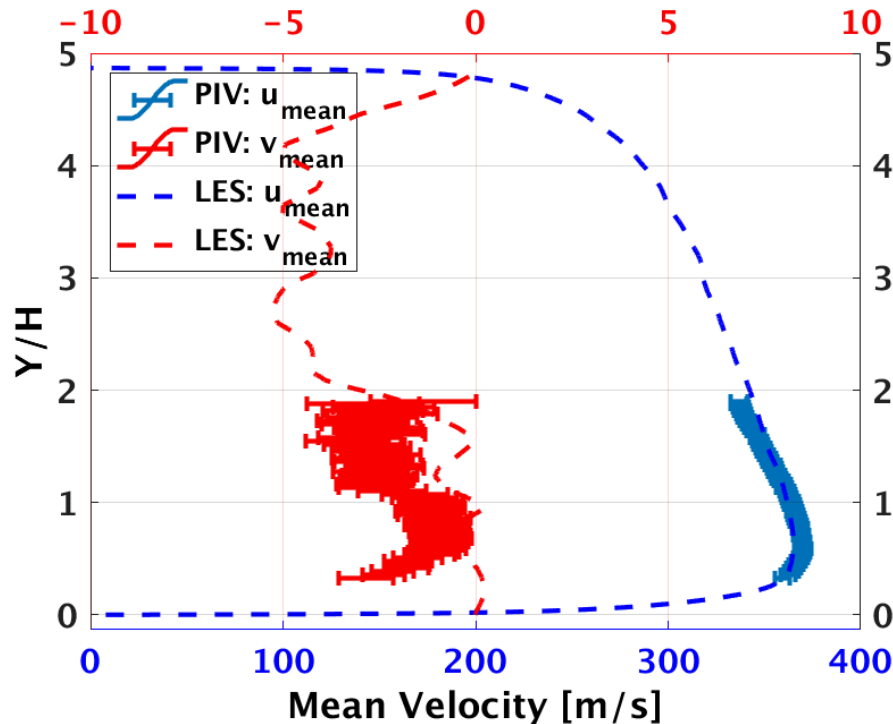
Mean and RMS Velocities, Integral Length Scales with PIV

- Mean velocities - Case 1 ($\Phi=0.44$, $M=0.6$)



PIV ↔ LES comparison

- Mean and RMS Profiles at DNS boundary: $X/H = -2.5$
- $M \sim 0.6$, $\Phi \sim 0.48$

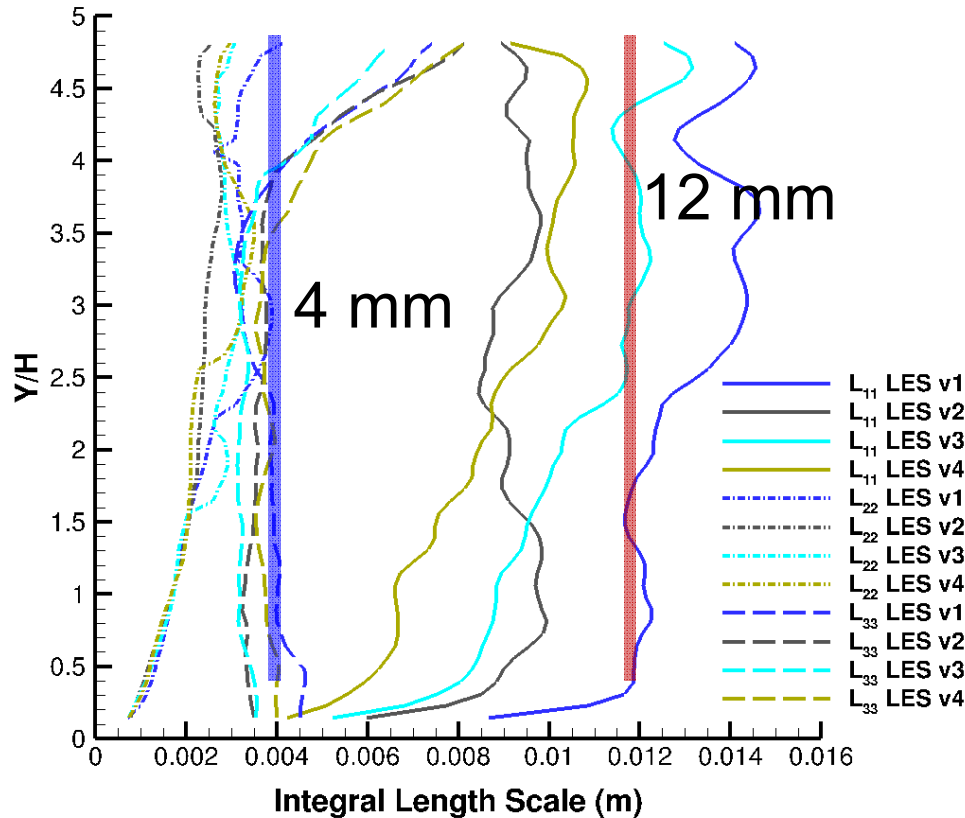


PIV ↔ LES comparison

- Integral length scales:

LES/RANS

PIV



Case	l_{11}	l_{22}
Max Φ , low M	TBD	TBD
Min Φ , high M	TBD	TBD
Min Φ , low M	TBD	TBD

Experimental data taken at the DNS B-C and $Y/H = 2$

OH PLIF Setup

OH PLIF setup

- Dye laser: 283.55 nm
- Laser sheet FWHM: 25 μm
- $f/2.8$ lens
- Mag. = 1.91
- FOV = **6.86 x 6.86 mm**
 - 512 x 512 pixels
 - 13.4 $\mu\text{m}/\text{pixel}$
 - after 2 x 2 binning
- **In-plane resolution (39 μm x 39 μm)**

Spatial filter for
thin laser sheet

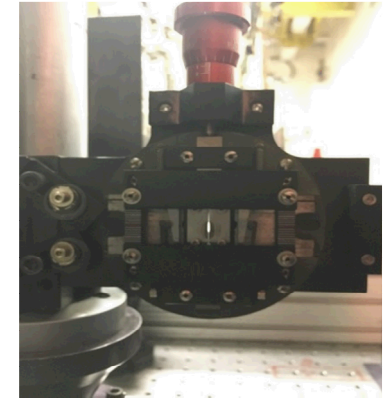
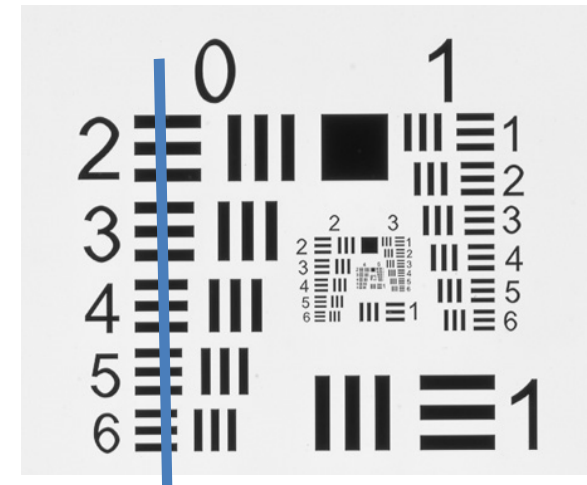
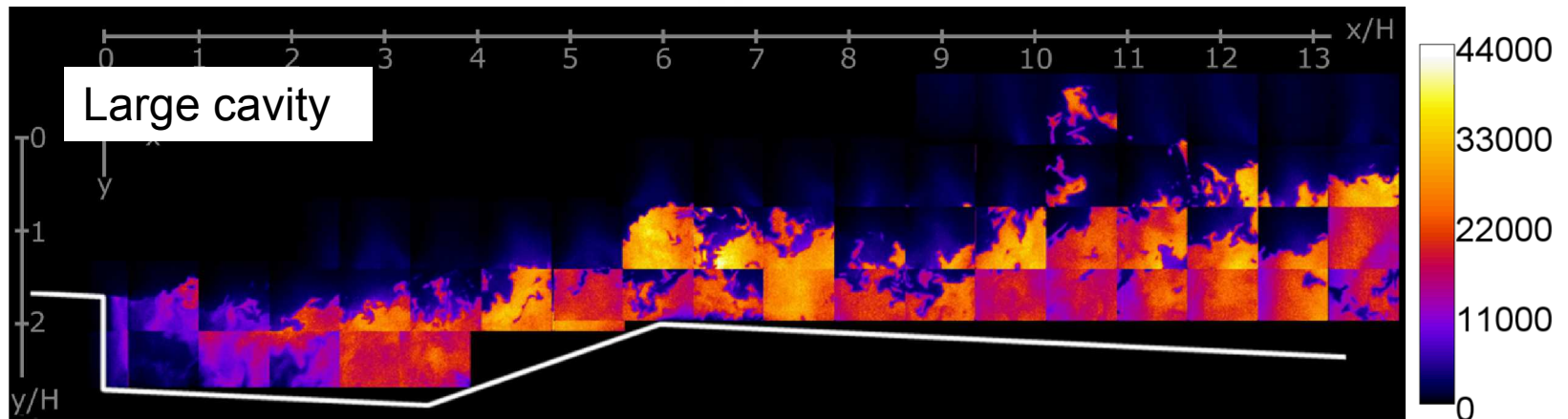
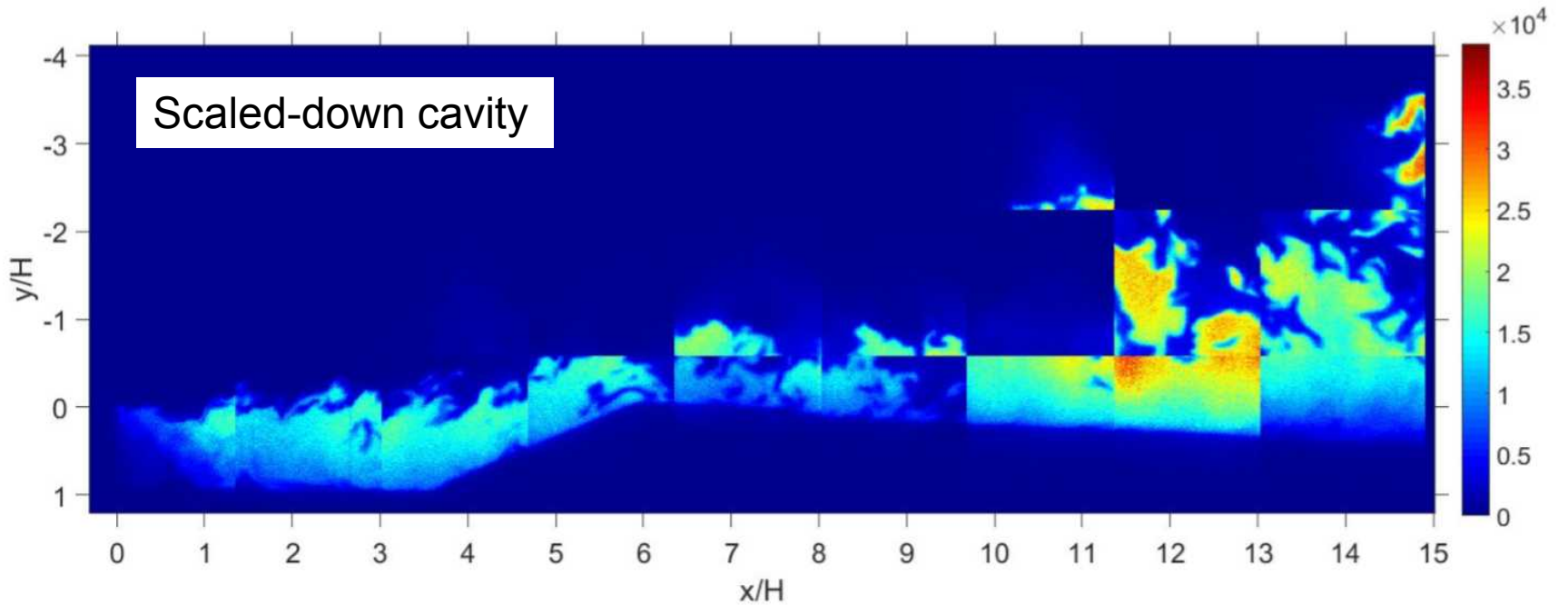


Image
resolution
analysis

USAF-1951 Resolution Target

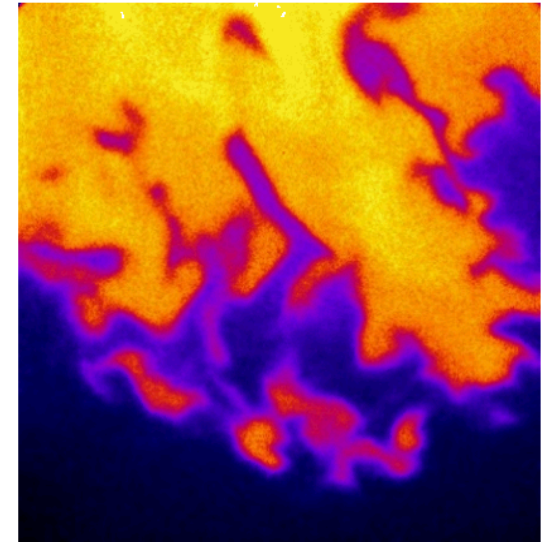
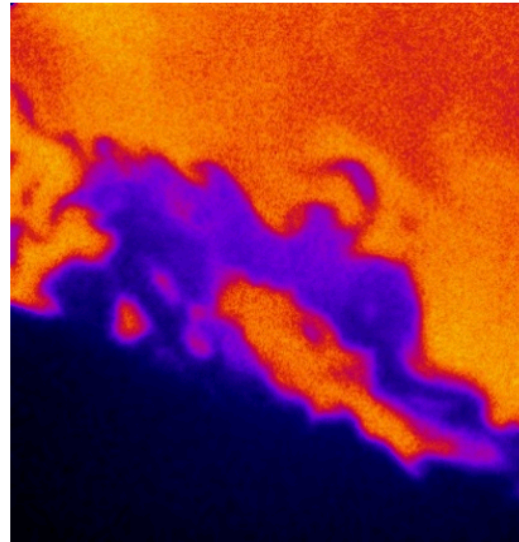
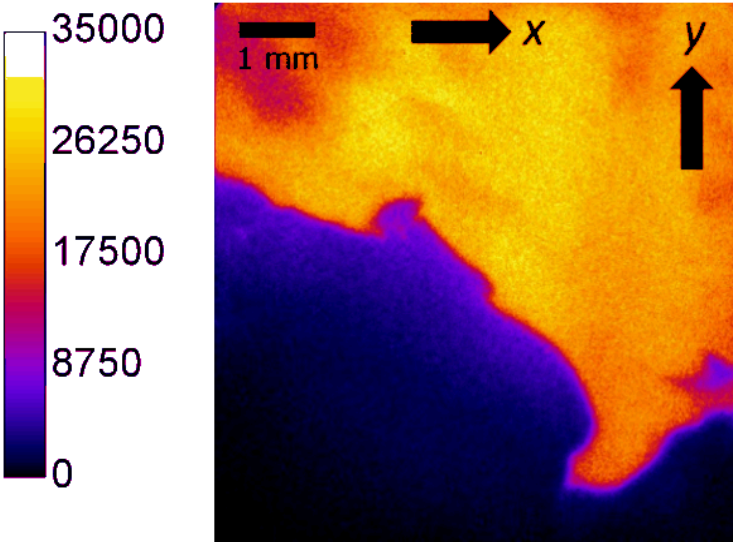
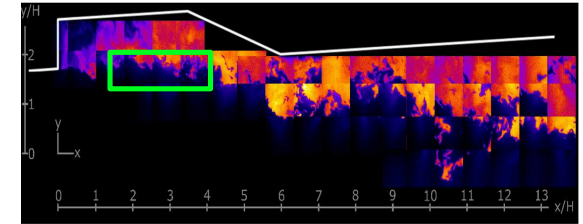


Compilation of Qualitative OH PLIF Data



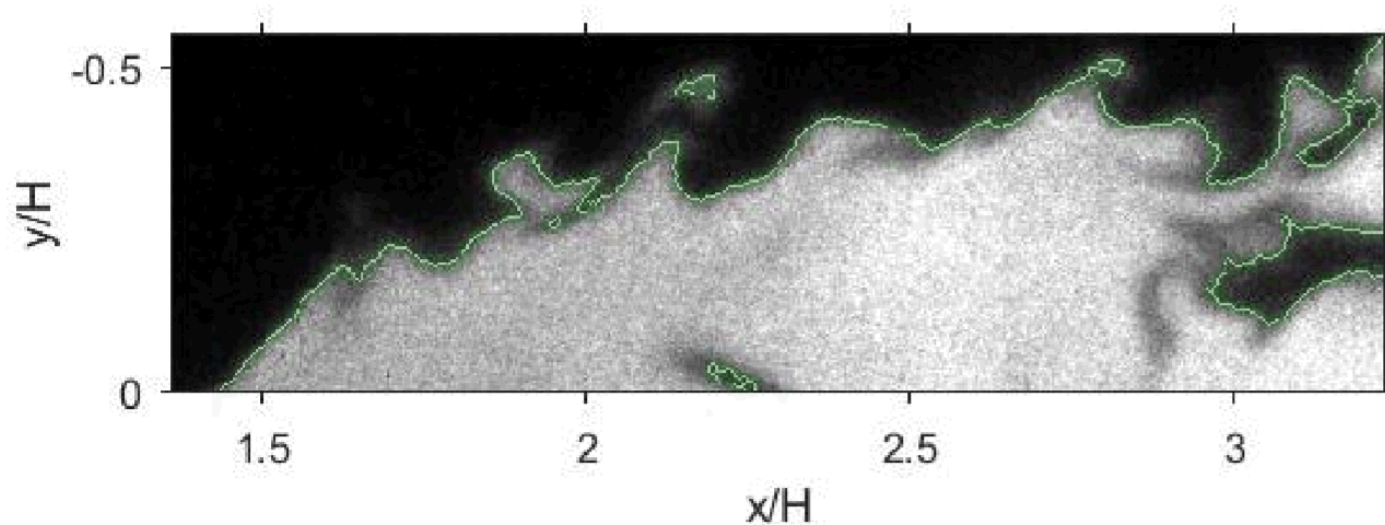
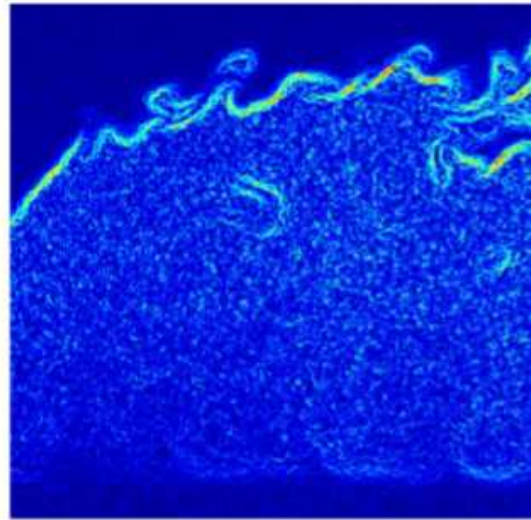
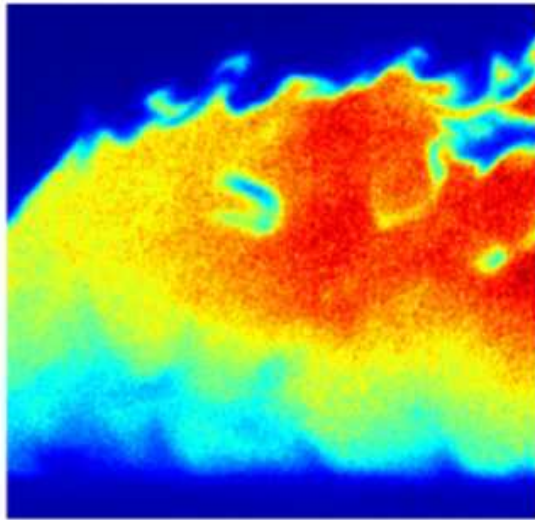
Instantaneous OH Images

- 200 images at each location in large cavity
- 1000 images at each location in small cavity

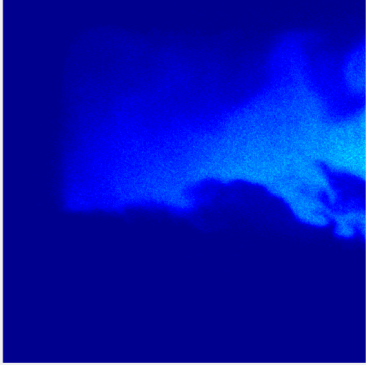


- Evidence of flamelet to distributed flame structures?
- 3D effects?

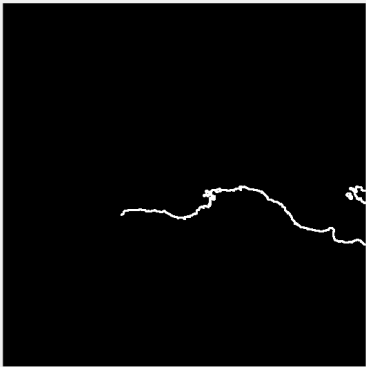
Flame Front Detection



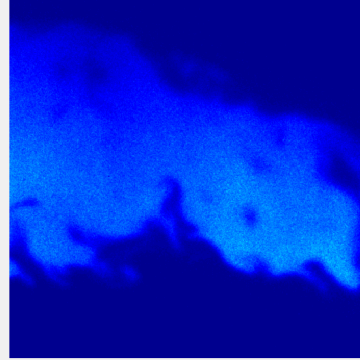
FSD – Single Images



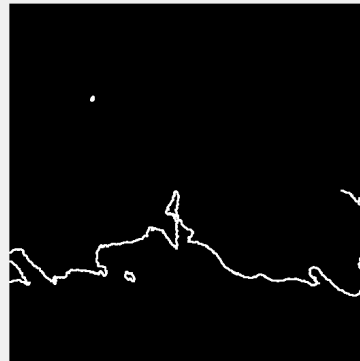
$x/H = 0.6226, y/H = 0.1429$



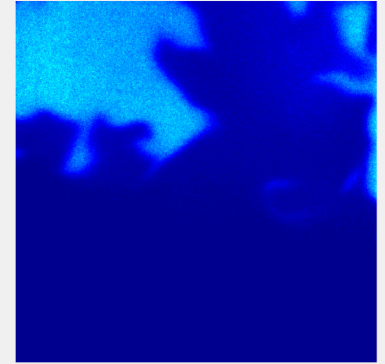
$FSD = 0.23639 \text{ mm}^{-1}$



$x/H = 3.9559, y/H = 0.1429$



$FSD = 0.50397 \text{ mm}^{-1}$

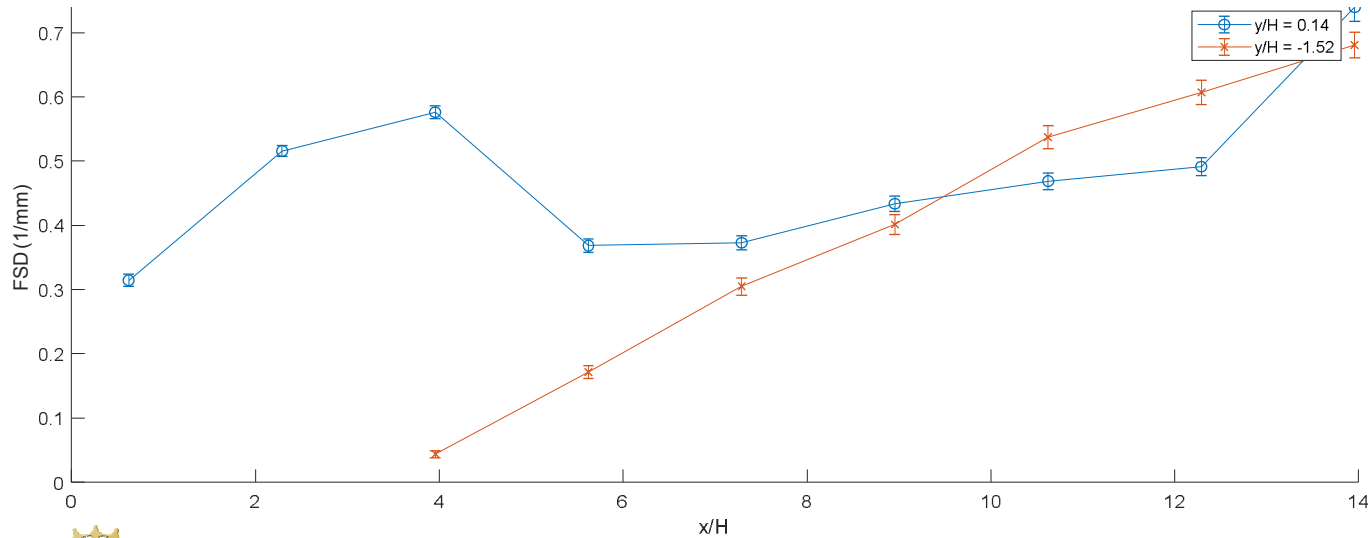
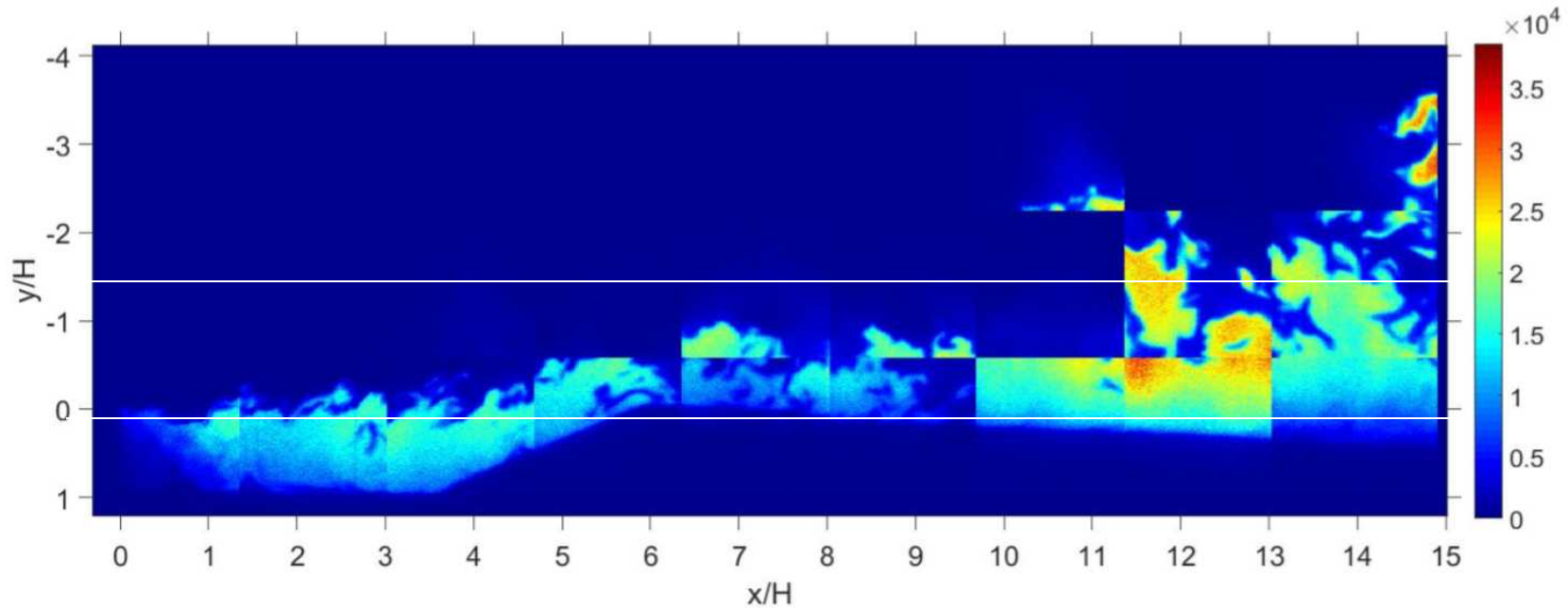


$x/H = 13.9559, y/H = -1.5238$



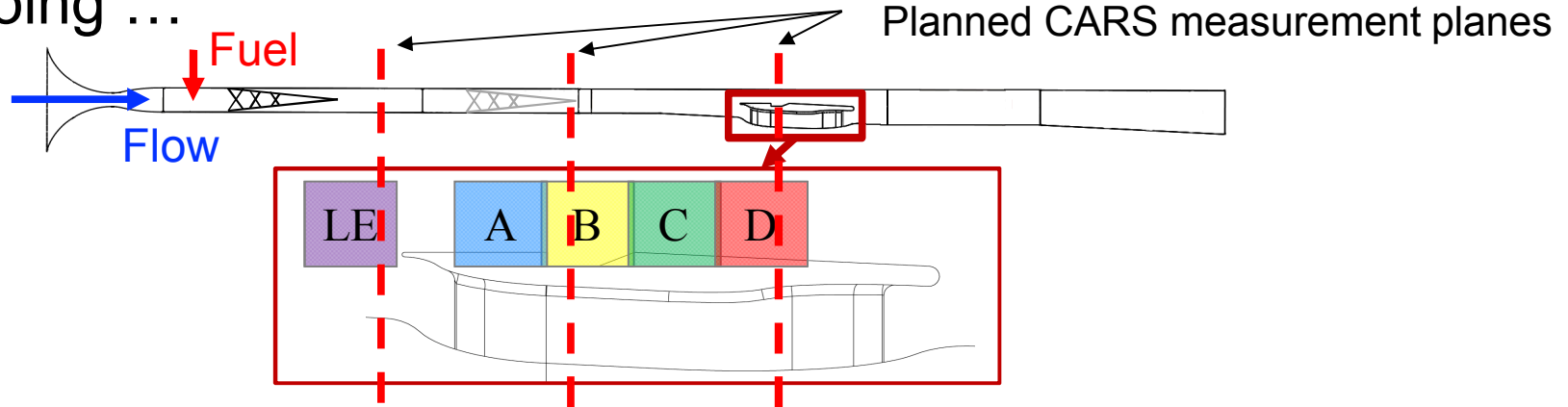
$FSD = 0.6366 \text{ mm}^{-1}$

Small cavity FSD trend

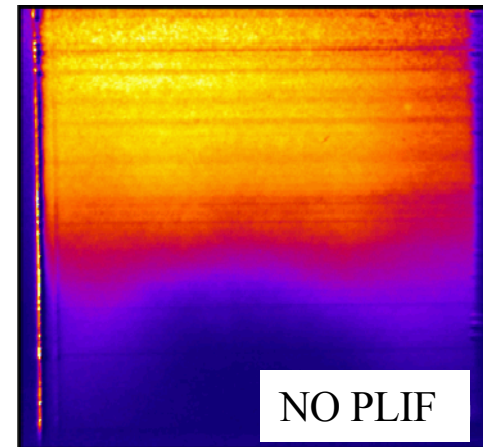
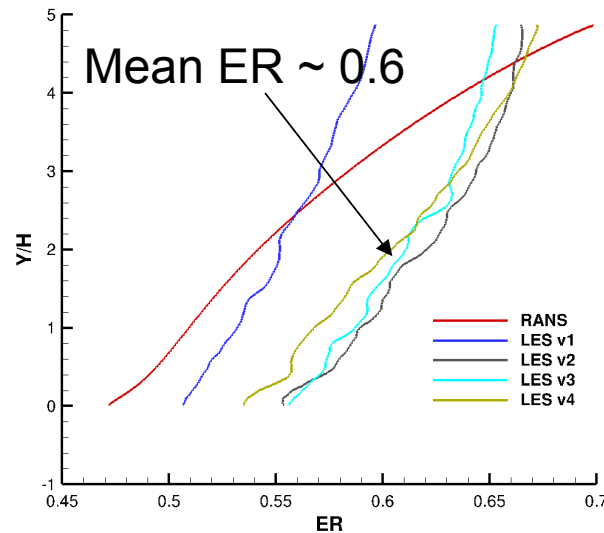


CARS Measurements of C₂H₄, T, and ...

- Quantification of fuel or ER stratification at DNS inflow plane is on going ...

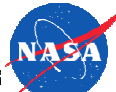


LES show ER variation of 0.55-0.65, consistent with previous NO-PLIF mixing studies

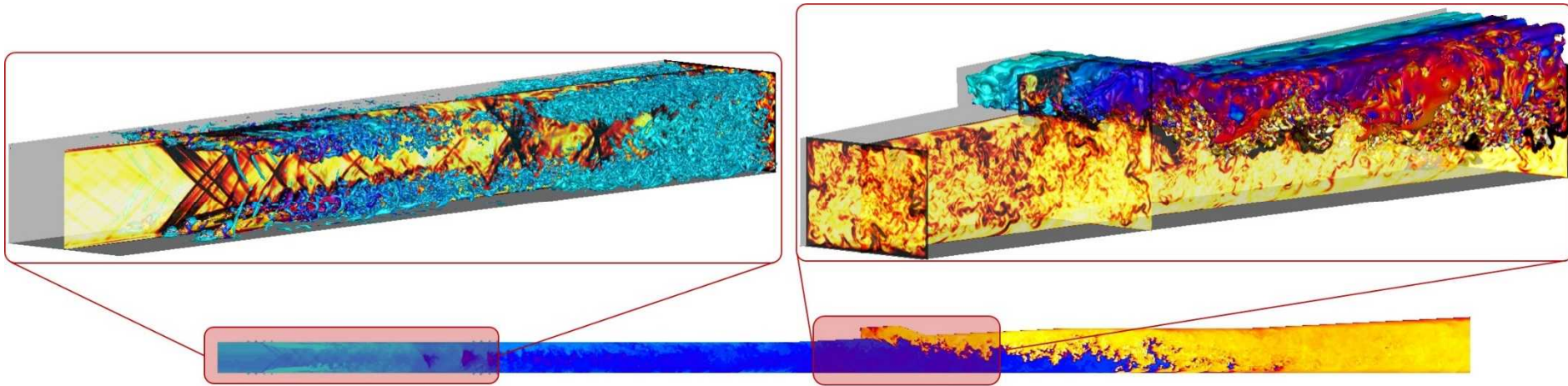


Simulations

- Full flow-path simulation using hybrid RANS/LES
- Reduced domain with DNS (mostly 2D)

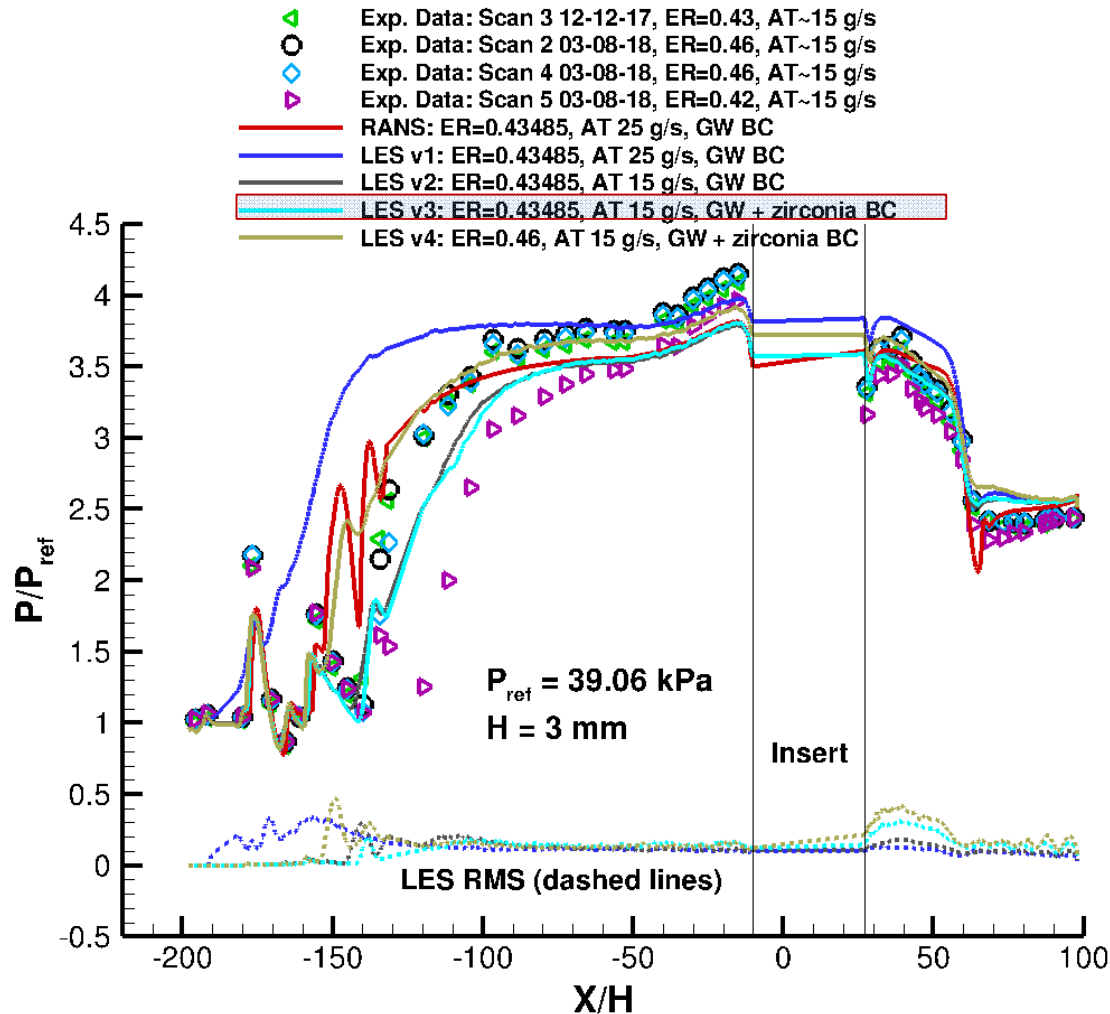


LES/RANS



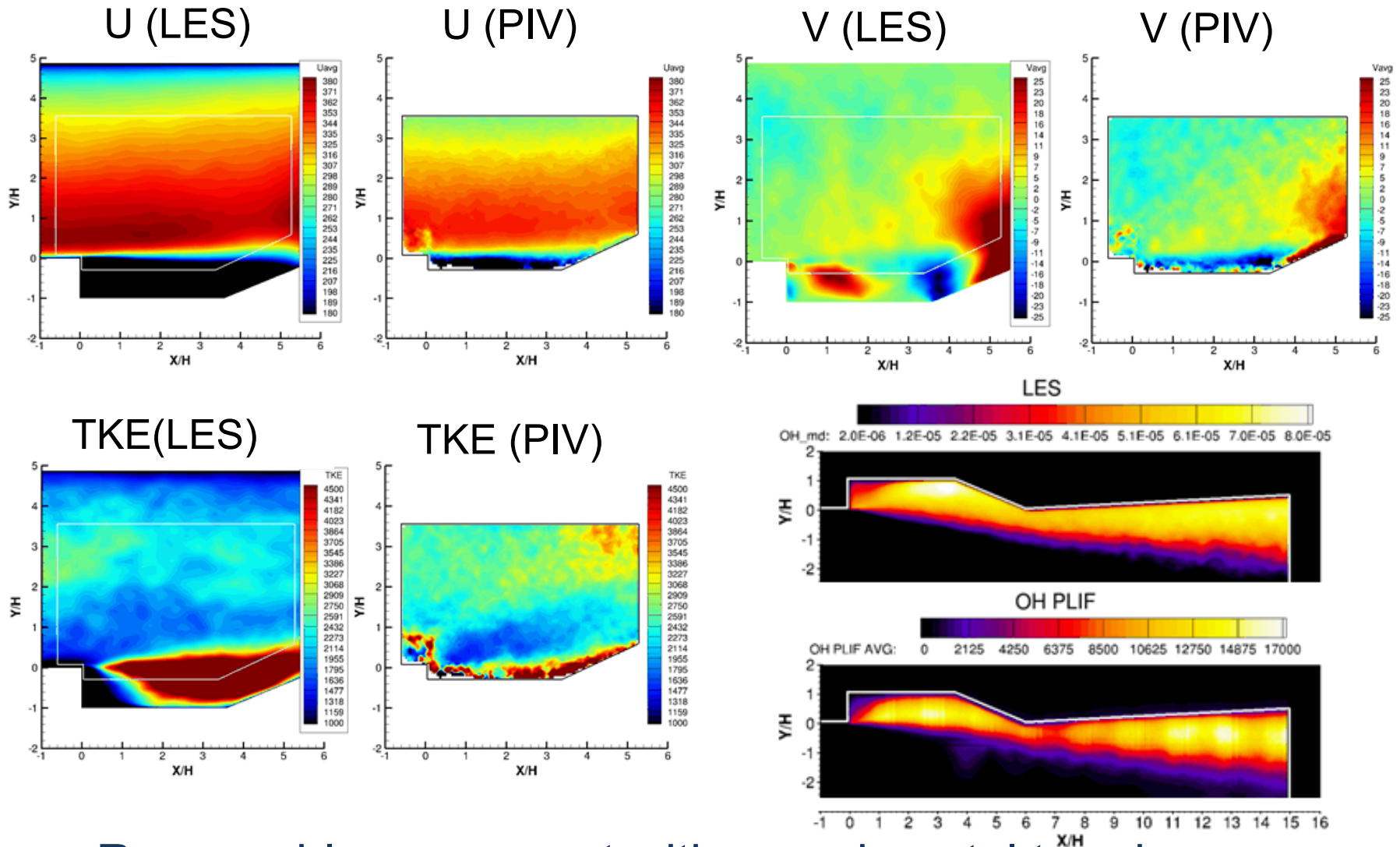
- Several simulations run on small cavity configuration
 - Varying inflow ER
 - Varying surface thermal boundary conditions (conjugate heat transfer models for zirconia-coated sections and glass sections)
 - Varying air-throttle settings (needed to choke flow)
 - 90 M cell mesh
 - TP-2 ethylene oxidation mechanism
 - Immersed-boundary rendering of flameholder strut (structured body-fitted meshes elsewhere)

LES/RANS – Wall Pressure



- Case v3 highlighted for subsequent comparisons

Velocity / OH Near Cavity



- Reasonable agreement with experimental trends

Flame Angle Calculation

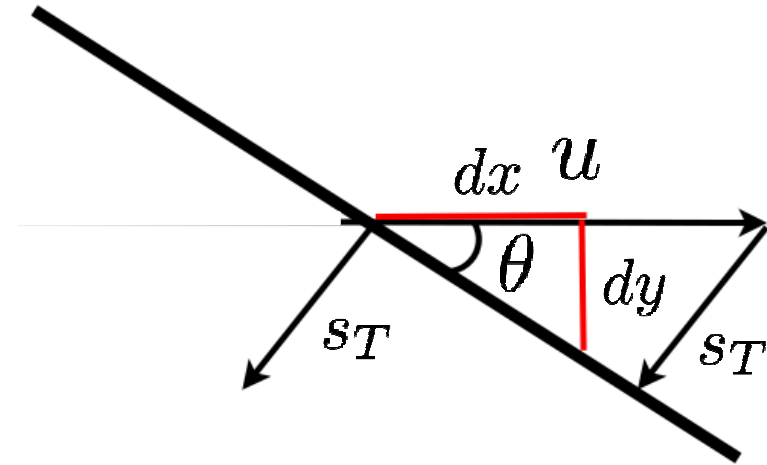
- Extract data upstream of flame:
 $ER, T, u, u', \text{ and } l_t$
- Compute laminar and turbulent flame speeds:

$$s_L(ER, T) \quad (\text{Brown and Lawn})$$

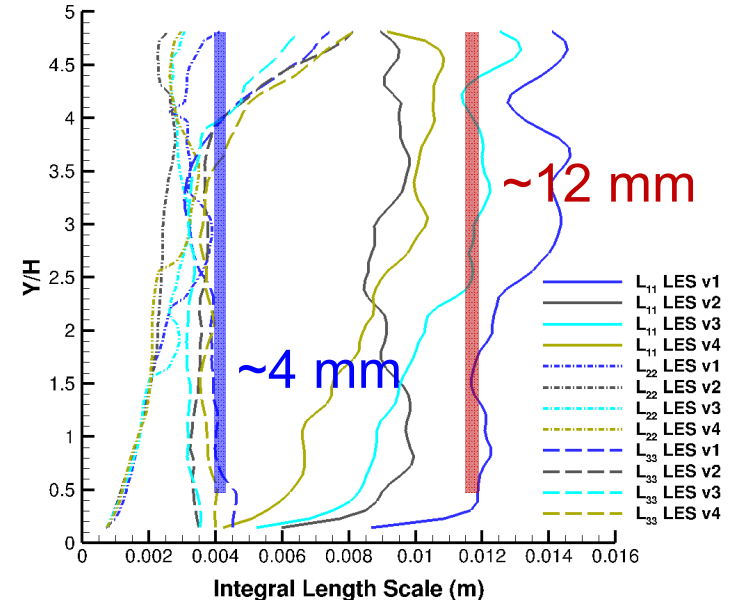
$$Re_t(u', l_t, s_L, l_F)$$

$$\frac{s_T}{s_L}(Re_t, u', s_L) \quad (\text{Zimont, Peters})$$

- Use geometric relations to compute flame angle and integrate to calculate flame front

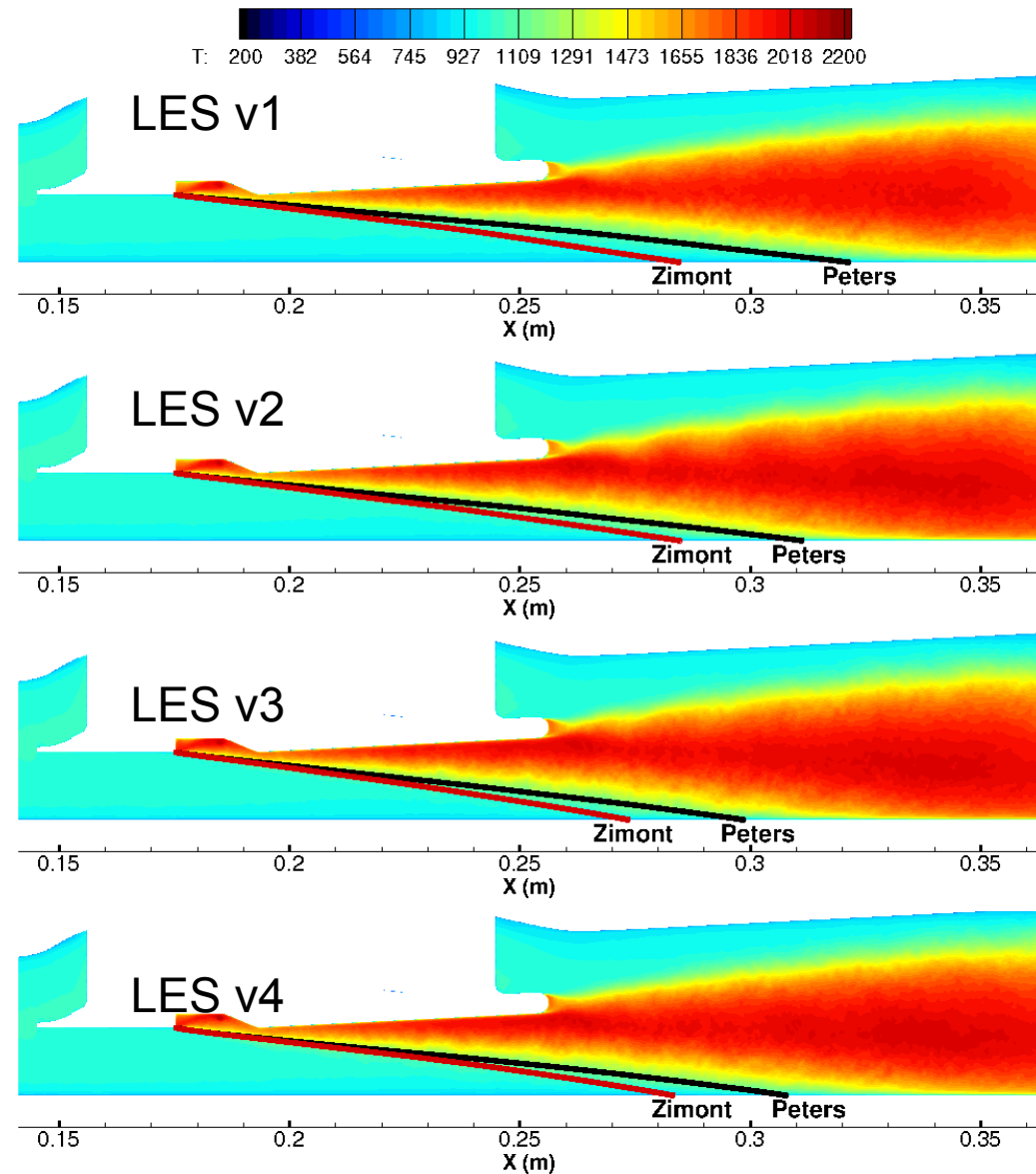


Integral length scales



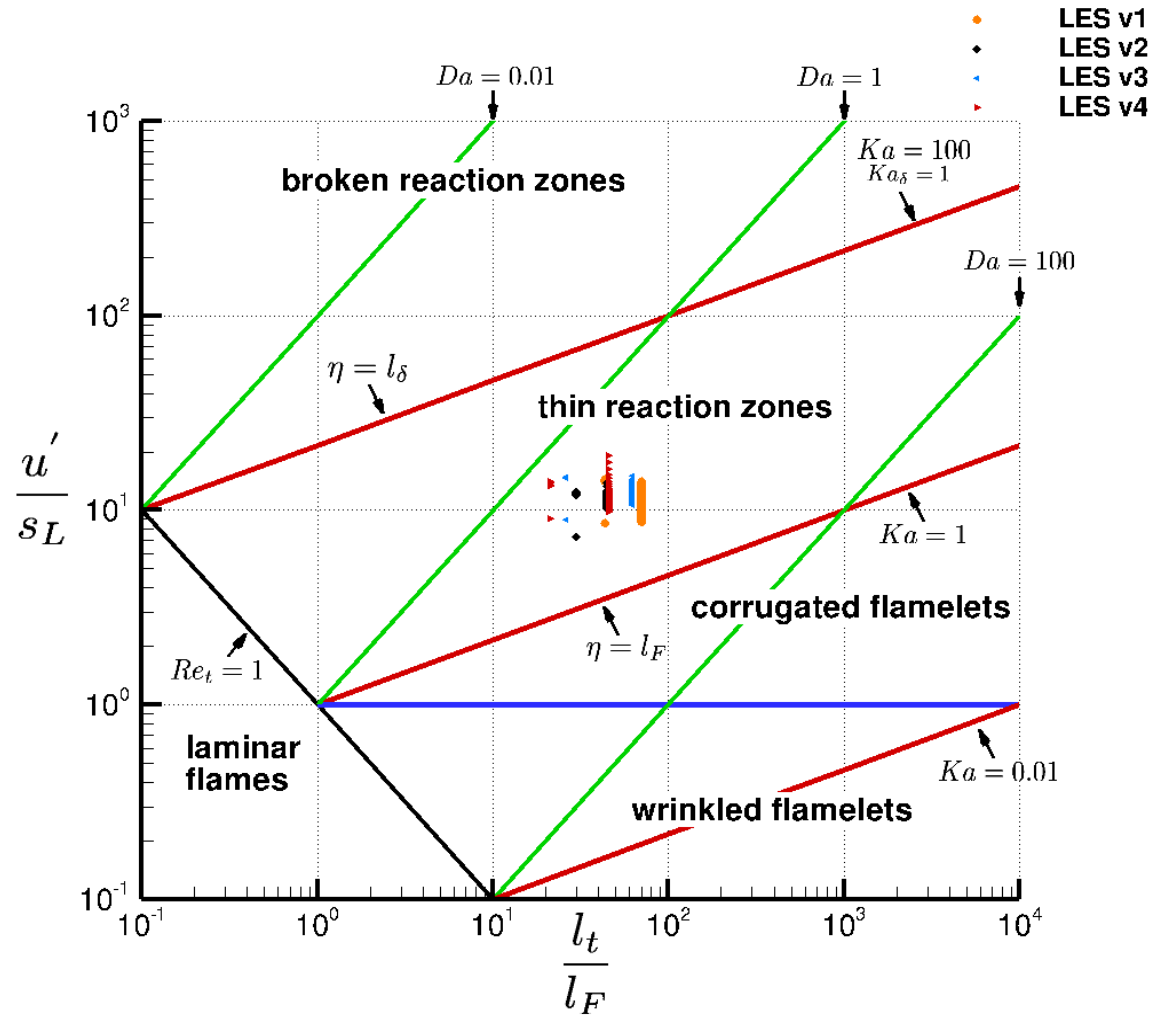
Flame Angle

- Excellent agreement with flame-front prediction using Peters flame-speed correlation
- LES v3 has the steepest flame angle (highest TKE levels and nearly the same local ER)
- LES v4 has a higher global ER, but not the highest local ER
- Shock train position influences TKE, mean velocity, and local ER distributions
- Cancellation of influences leads to little variation in flame angle



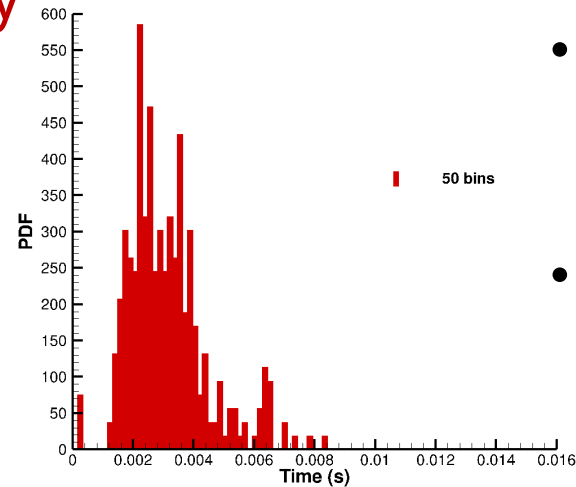
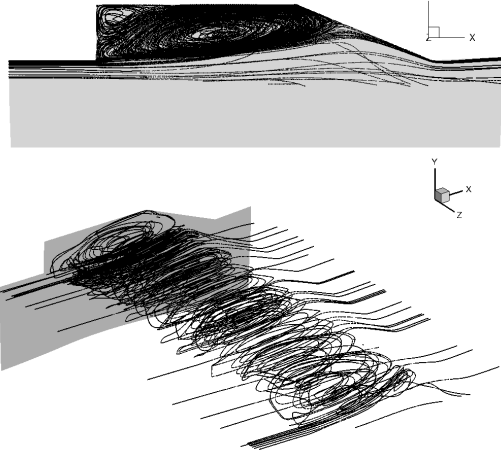
Regime Diagram: Small Cavity

- Data extracted upstream of flame
- Axial integral length scale used
- CANTERA used to estimate flame thickness
- Thin reaction zones regime is clearly prevalent (also true for large cavity configuration)



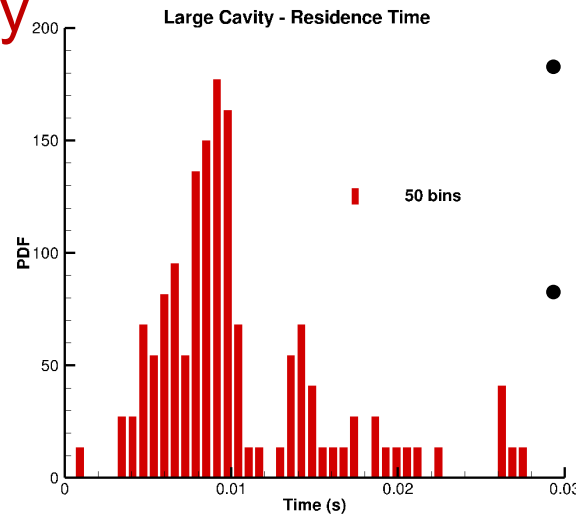
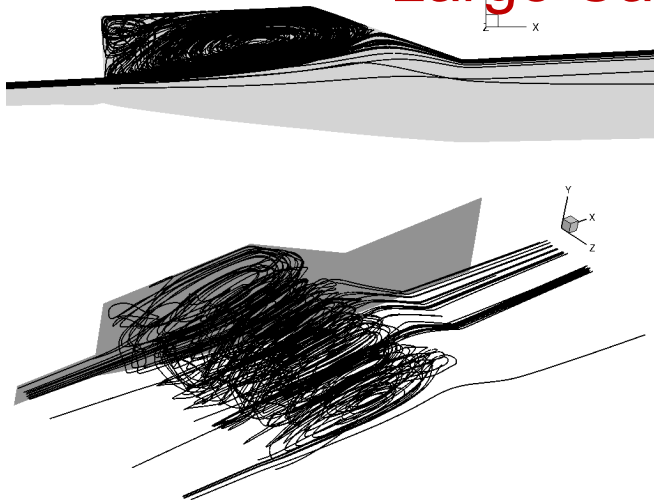
Cavity Residence Time Distributions

Small Cavity



- Average residence time: ~3.12 ms
- Most probable residence time: ~2.22 ms

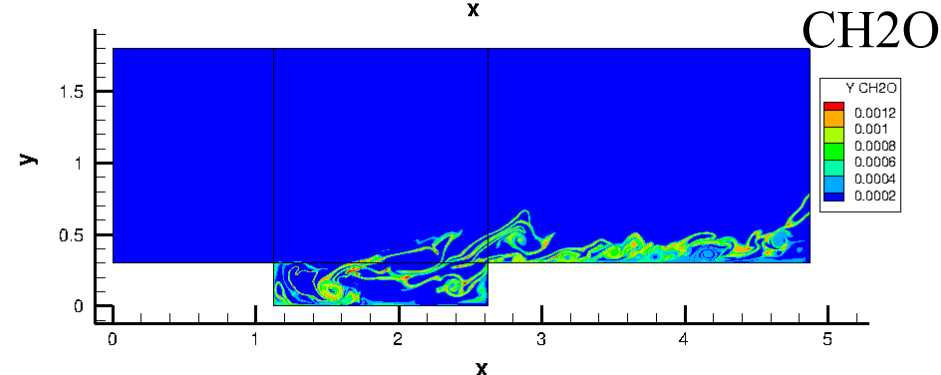
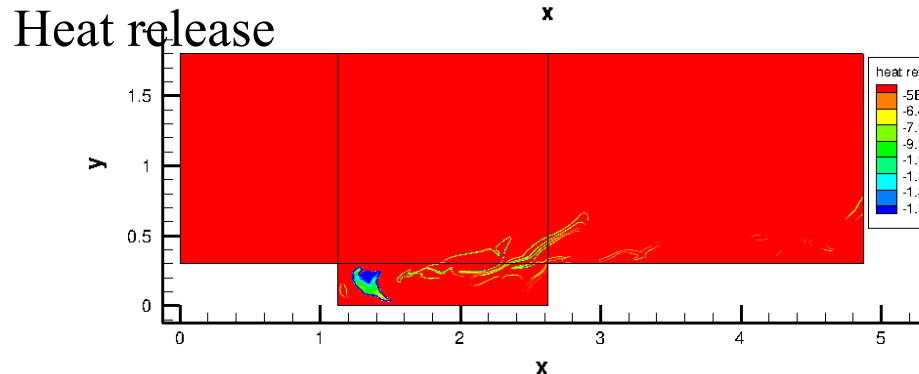
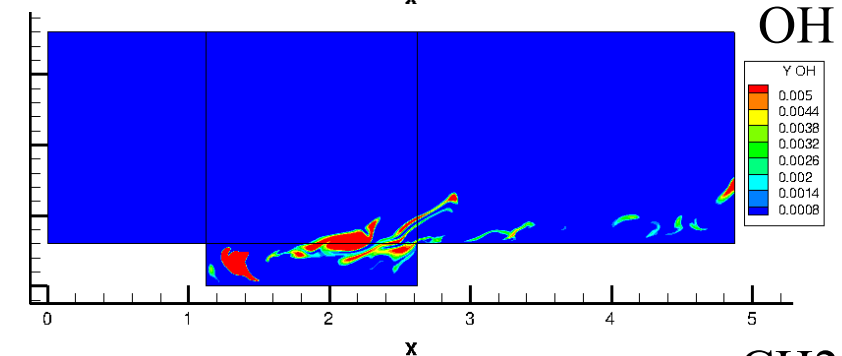
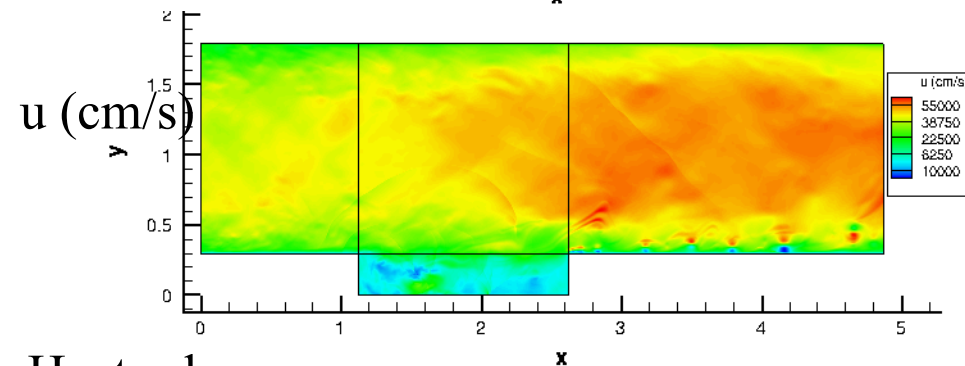
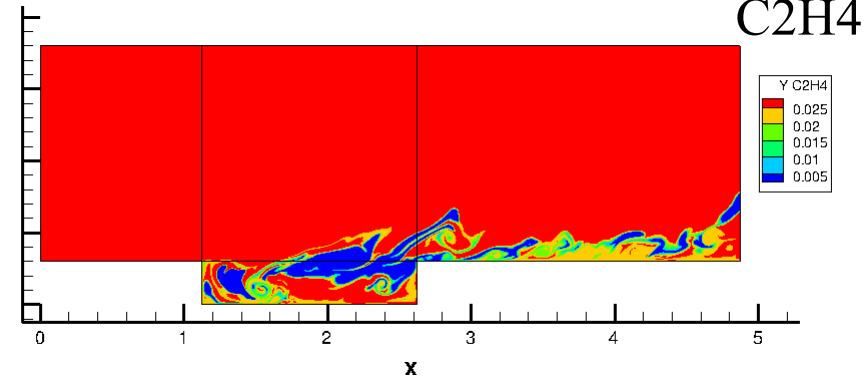
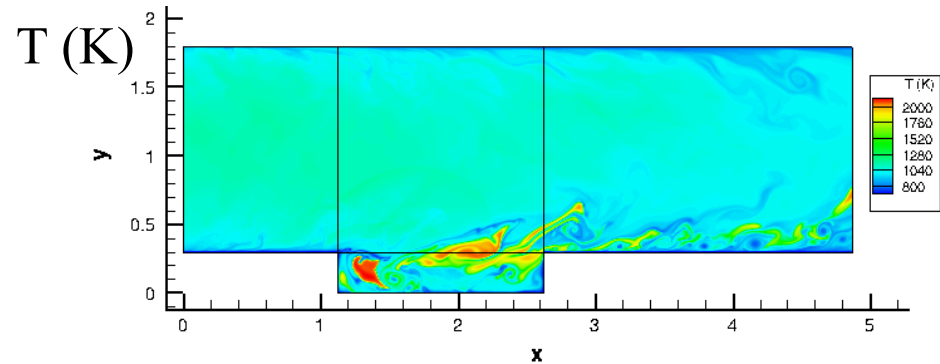
Large Cavity



- Average residence time: ~10.8 ms
- Most probable residence time: ~9 ms

DNS with Scaled Down Rectangular Cavity

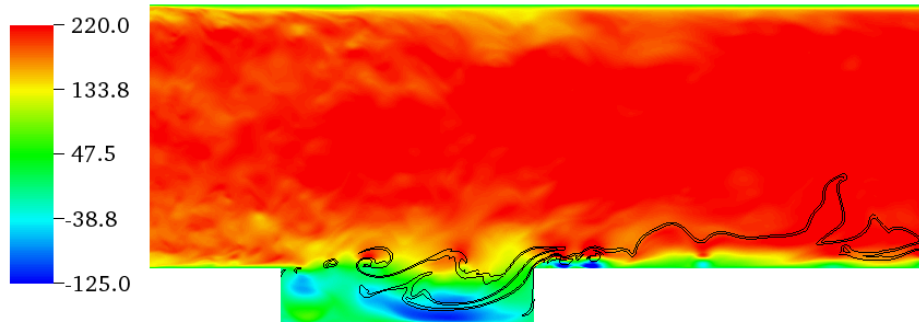
- $L/D=6$, $M=0.6$, $\phi=0.42$, $T_s = 1125K$, $p_s = 1.7$ atm



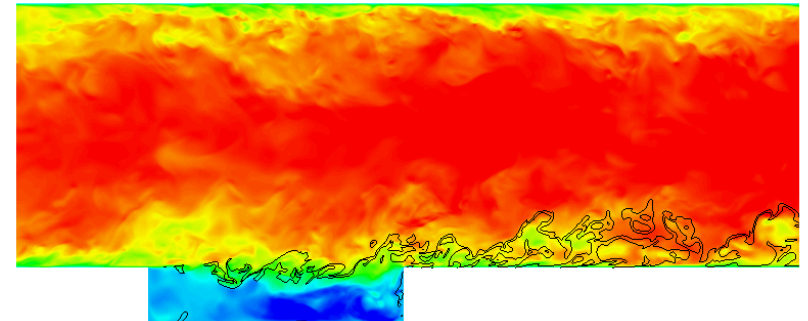
DNS with Scaled Down Rectangular Cavity

- Significant differences in turbulence and flame structure between 2D and 3D simulations at: $M=0.3$, $\phi=0.42$, $T_s = 1125\text{K}$, $p_s = 1.72\text{ atm}$

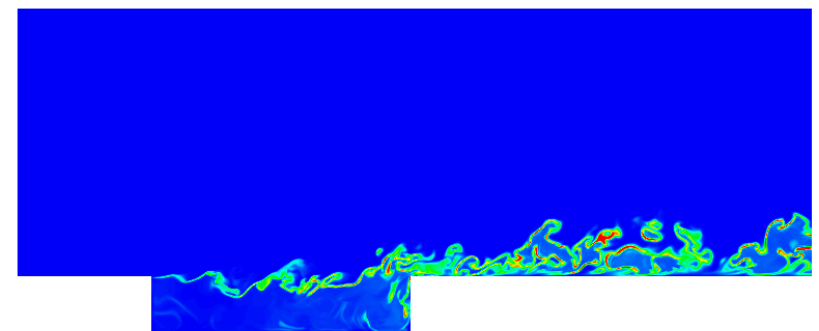
2D



3D

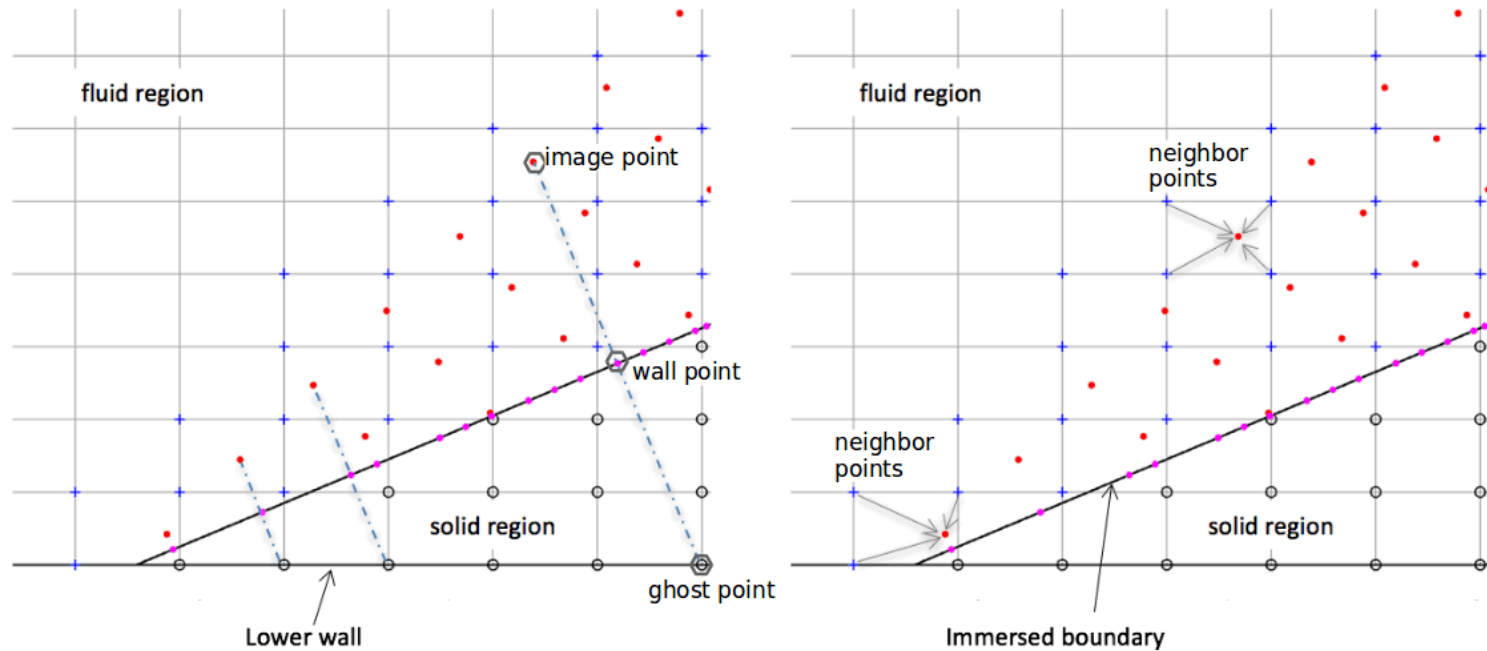


- Stream-wise velocity [m/s] contour plots with black-line indicating peak heat release. Turbulence decays away from inlet.



- Heat release rate [$\text{J/m}^3/\text{s}$] contour plot, flame is significantly more wrinkled in 3D case.

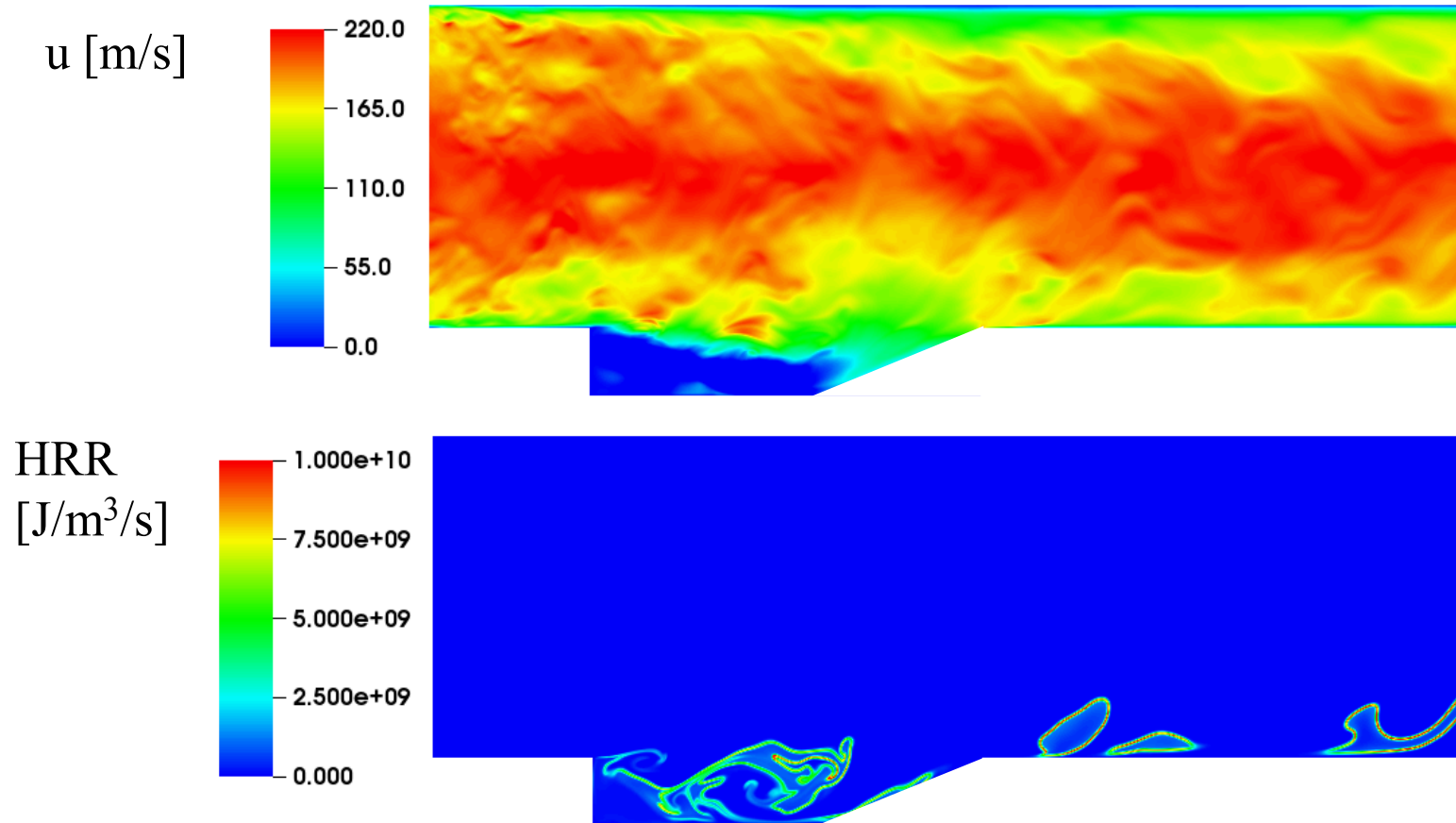
DNS with Immersed Boundary Method



- IBM allows for non-mesh conformal geometries to be simulated, such as the linear-close up ramp
- A ghost zone approach is taken (Parnaudeau et. al., 2004)
- Stencil formed across image, wall and ghost point
- Wall and ghost points obtained from physical BC's
- Image points obtained by Inverse Distance Weighted interpolation

DNS with Immersed Boundary Method

- DNS with linear close-up ramp simulated in 2D
- Conditions: $M=0.3$, $\phi=0.42$, $T_s = 1125\text{K}$, $p_s = 1.72\text{ atm}$



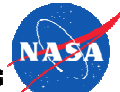
Summary of Accomplishments

- Demonstrated that 3D printed, 1/3 scale cavity with a premixed ethylene-air mixture can flame hold at $M=0.65$ conditions
- Inflow velocity B.C.'s for the DNS domain has been characterized with $u_{\text{mean}} = 370$ m/s, turb. intensity of about 12%, $l_{11} = 12$ mm, $l_{22} = 4$ mm
- OH imaging with resolution of $39 \times 39 \times 25$ microns have revealed fine scale structure corresponding to high Ka #
- LES simulations have revealed large scale flame dynamics, wall pressure comparisons, and key inflow conditions for the DNS domain
- S3D code has been used to analyze 2D vs 3D effects [rectangular cavity at $M=0.3$ and 0.6] and higher-order immerse-boundary method has been implemented for linear close-up ramp simulations



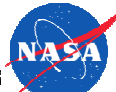
Ongoing Near Term Work ...

- Characterization of local ER with CARS (i.e. degree of stratification), turbulence statistics in flame region, ...
- High-resolution CH₂O, CH, ... with different excitation wave lengths and optics are on-going, with collaboration of Cam Carter at AFRL
- Full 3D DNS with linear close-up ramp needs HPC time, at a minimum 75 MCPU hrs
- RANS/LES analysis of resolved spectra, both velocity and scalar correlations, test turbulence-chemistry models, ...



Long Term Challenges ...

- Wall boundary conditions, especially the wall temperature/heat transfer (Danehy), wall roughness, edothermic cooling, ..
- High-resolution velocity (tomographic PIV – Lin Ma), particle-free methods (Gamba, Danehy, Cutler), ...
- Scalar correlations (line-CARS - Dedic), ...
-



Acknowledgements

- **PhD Students:**

- ✧ Clayton Geipel (UVa) with Cutler, Danehy, Chelliah
- ✧ Damien Lieber (UVa) with Goyne
- ✧ Tanner Nielsen (NCState) with Edwards
- ✧ Andreas Rauch (UVa) with Chen, Chelliah

- **UG Students:**

- ❖ Vanessa Awate, Walker Smith (UVa) with Chelliah
- ❖ Noah xxx (GWU) with Cutler

- **Research staff:**

- ✧ Dr. Aditya Konduri (Sandia National Lab) with Chen

***AFOSR-NSF Turbulent Combustion Program, with Dr. Chiping Li
and Dr. Song-Charn Kong as the technical monitors***

NSF DCL and REU Program



Sandia
National
Laboratories



NC STATE UNIVERSITY



Backup



Sandia
National
Laboratories

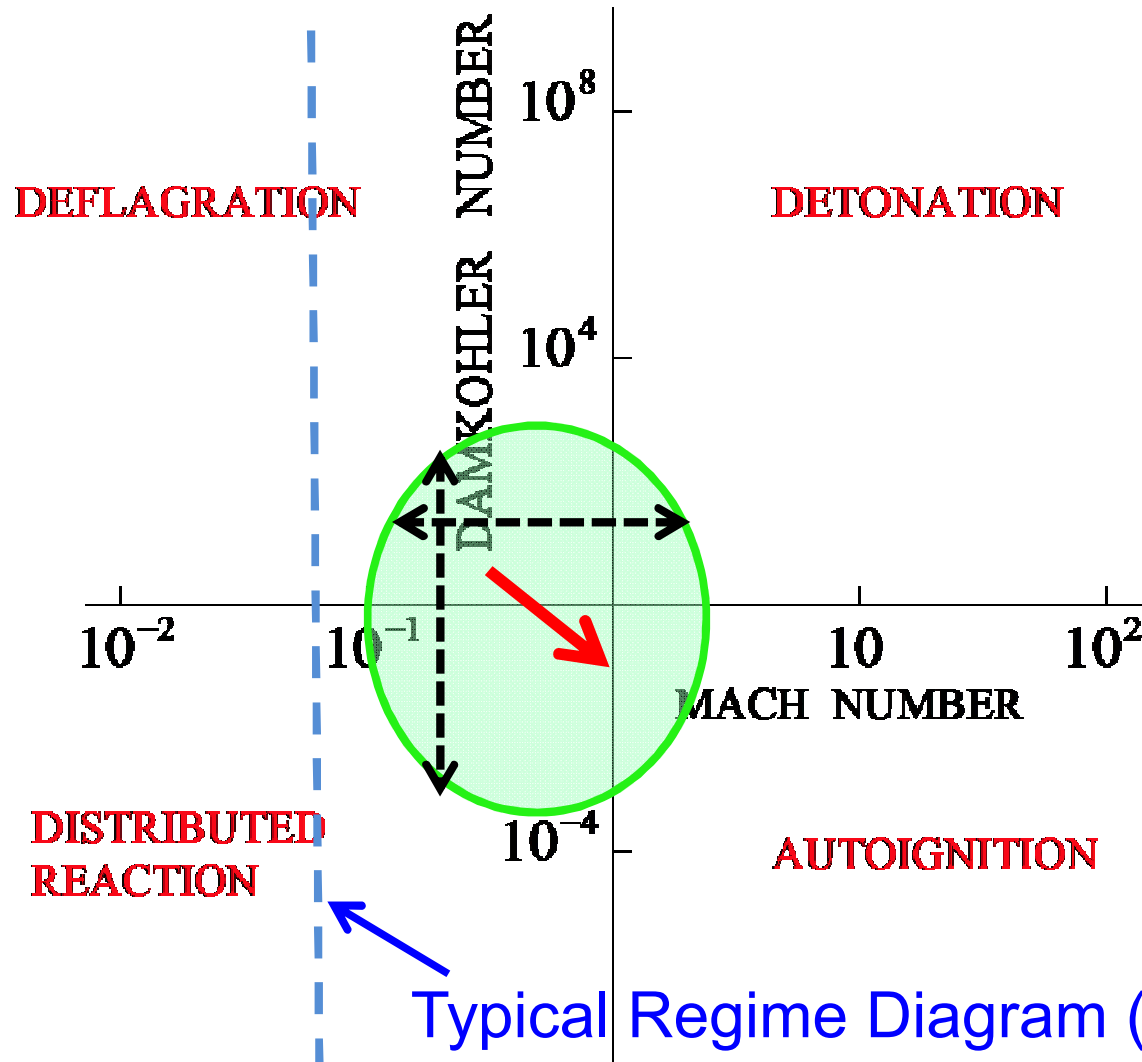


NC STATE UNIVERSITY



Ma-Da Regime Diagram (Williams, 2014)

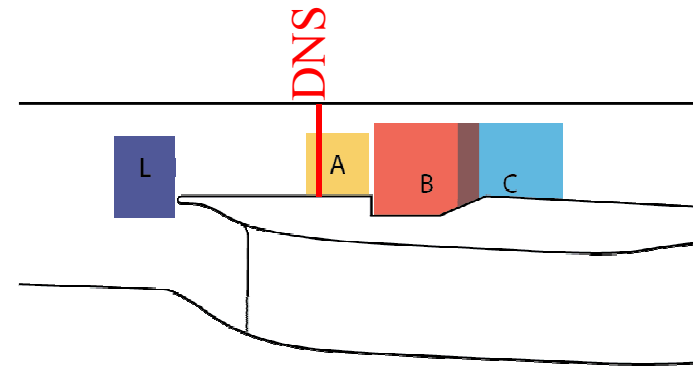
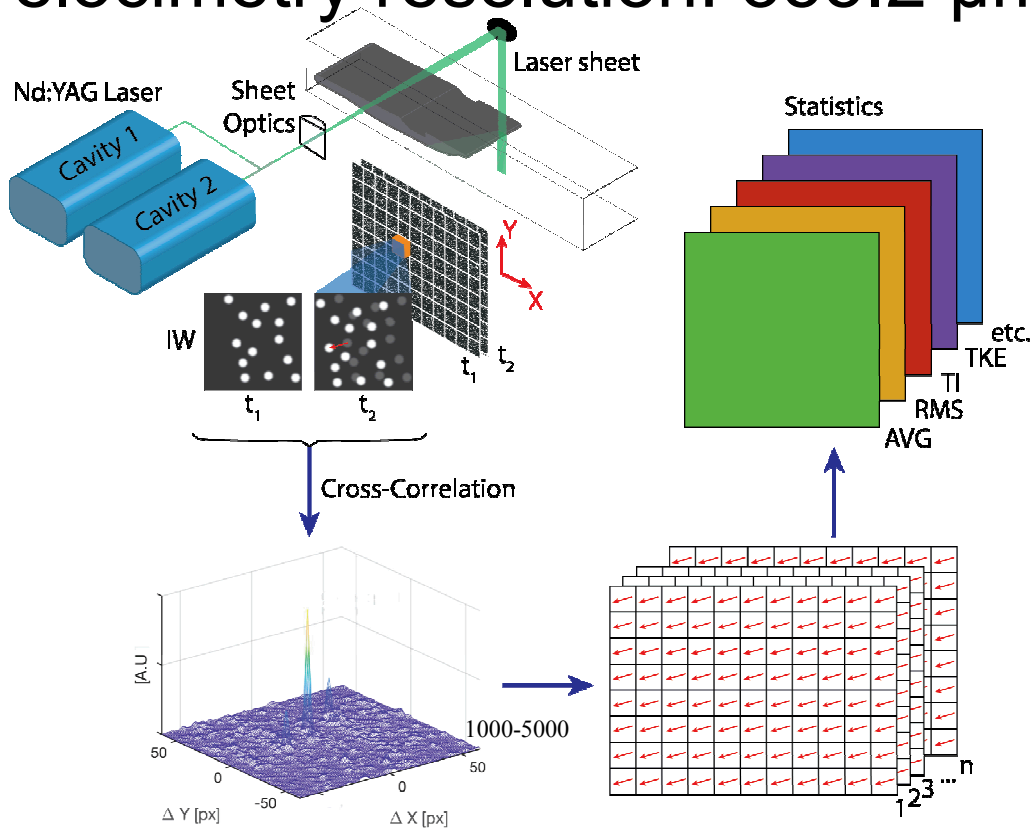
(Turbulent Combustion Workshop on Interaction between Scales, San Antonio, TX, 4/2014)



Typical Regime Diagram (Da, Re slice)

2D-2C PIV setup

- Measurement volume: $12 \times 9 \times 0.140 \text{ mm}^3$
- Smallest IW size: 48 px
- Velocimetry resolution: $355.2 \mu\text{m}$

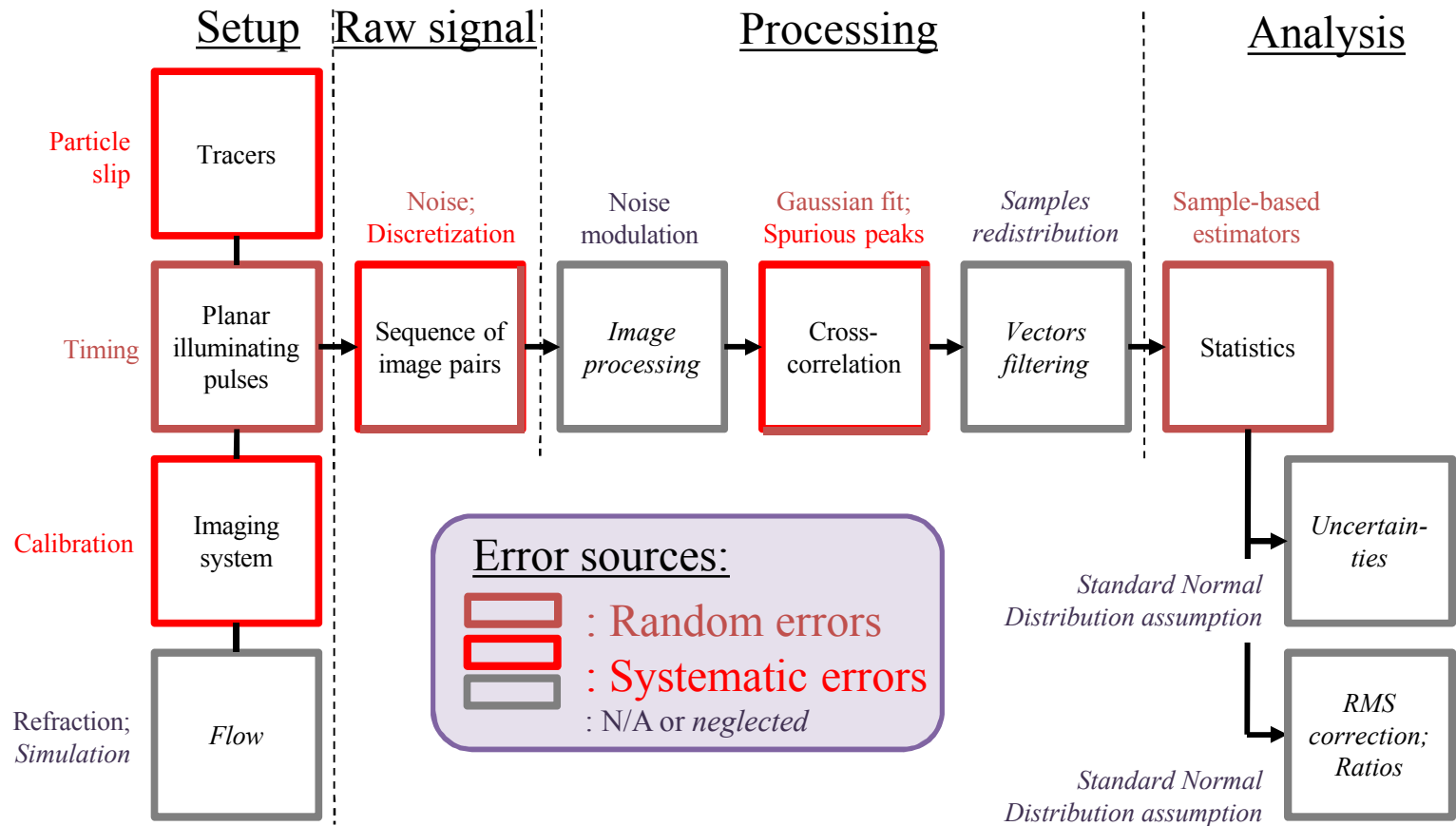


Cross-Correlation Map & Peak Selection
Displacement $\rightarrow$ Velocity

Vector Fields Stack

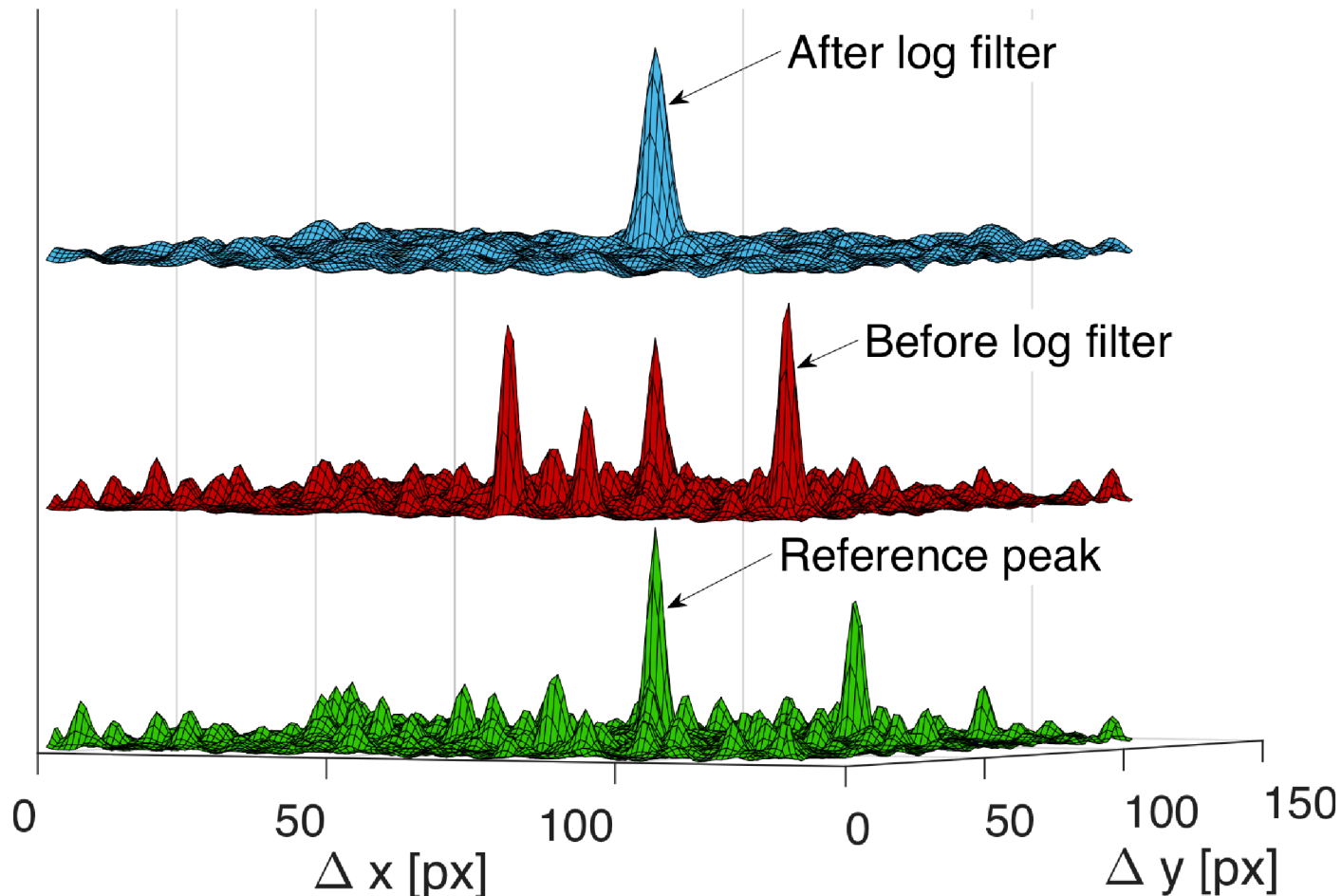


Sources of PIV uncertainties



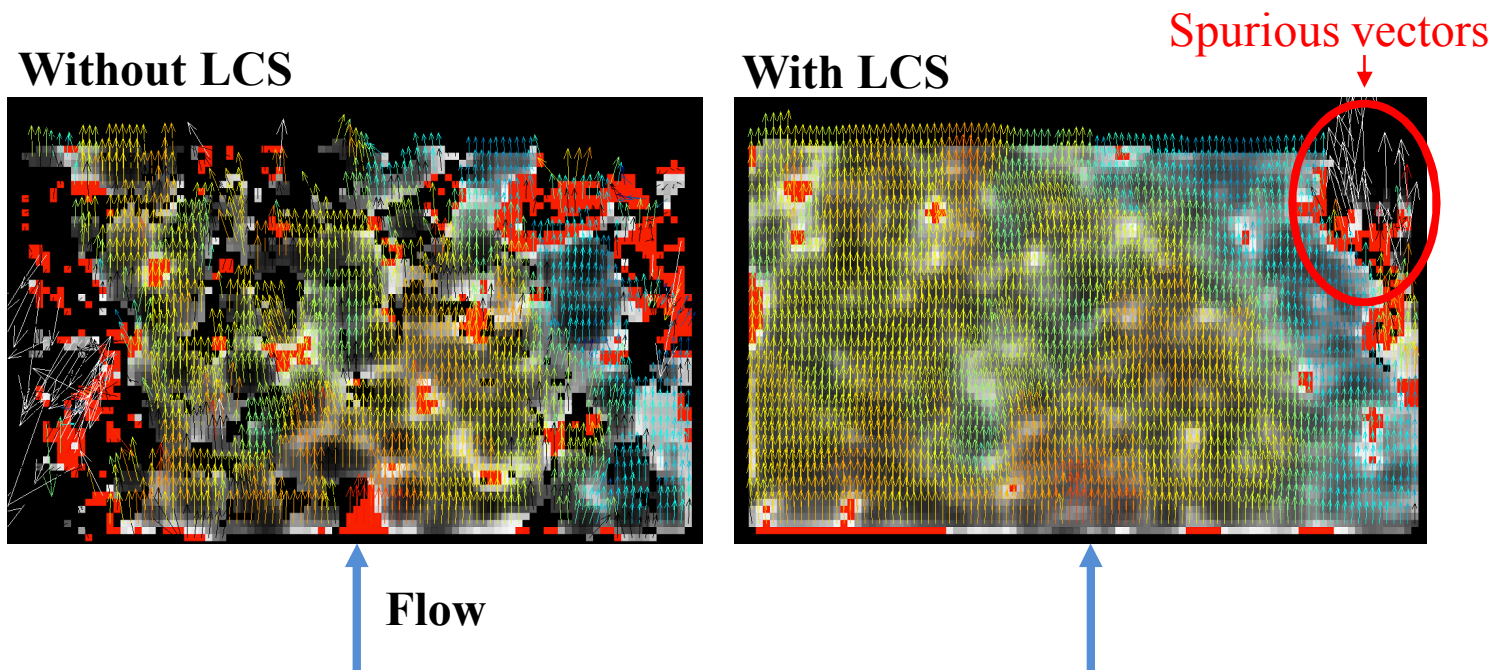
Effect of LCS pre-processing

Correlation maps for 2 rotating particles:



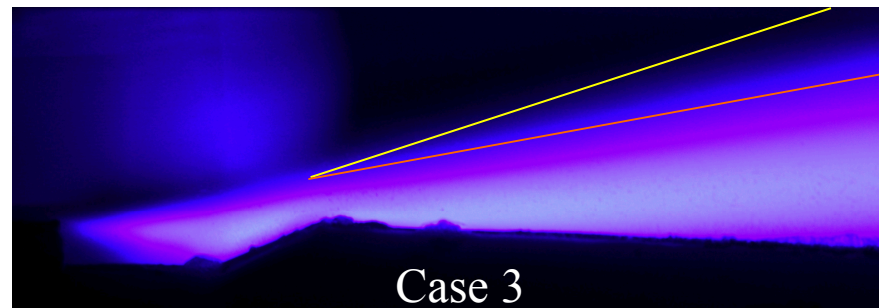
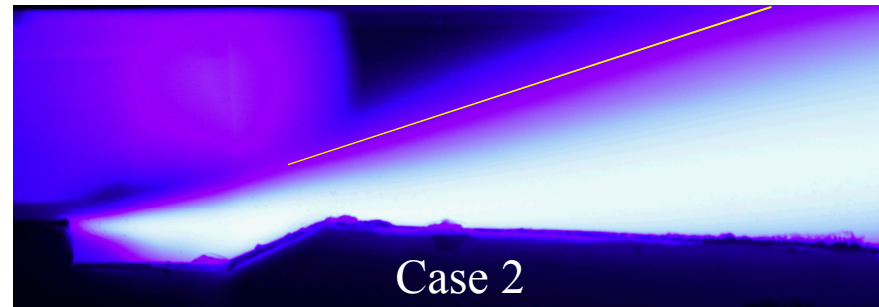
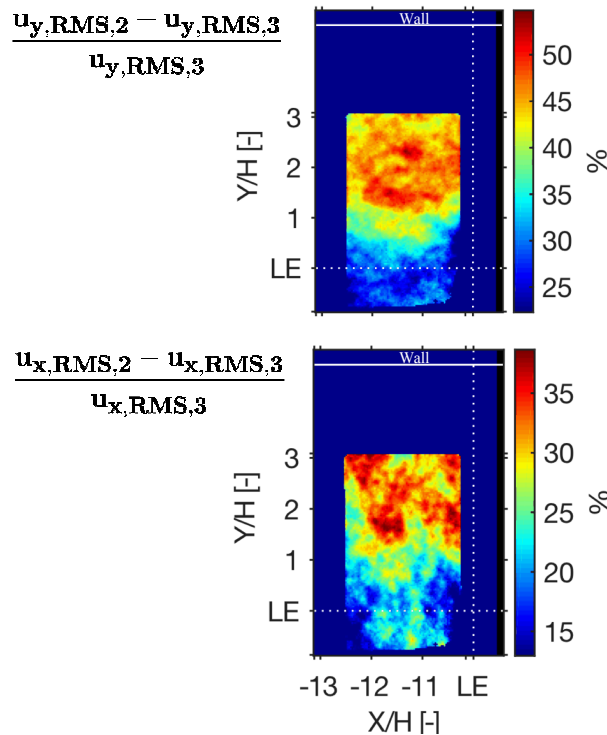
Effect of LCS pre-processing

- Good vectors remain but most of the spurious vectors are replaced by correct ones.
- Some post-processing still required (see red circle)



Comparison of case 2 (min Φ , max M) and case 3 (min Φ , min M)

- Median increase in $u_{x,RMS}$: 41% ; in $u_{y,RMS}$: 26%; uncertainty $\pm 10\%$.

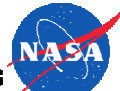


Flame Structure Analysis

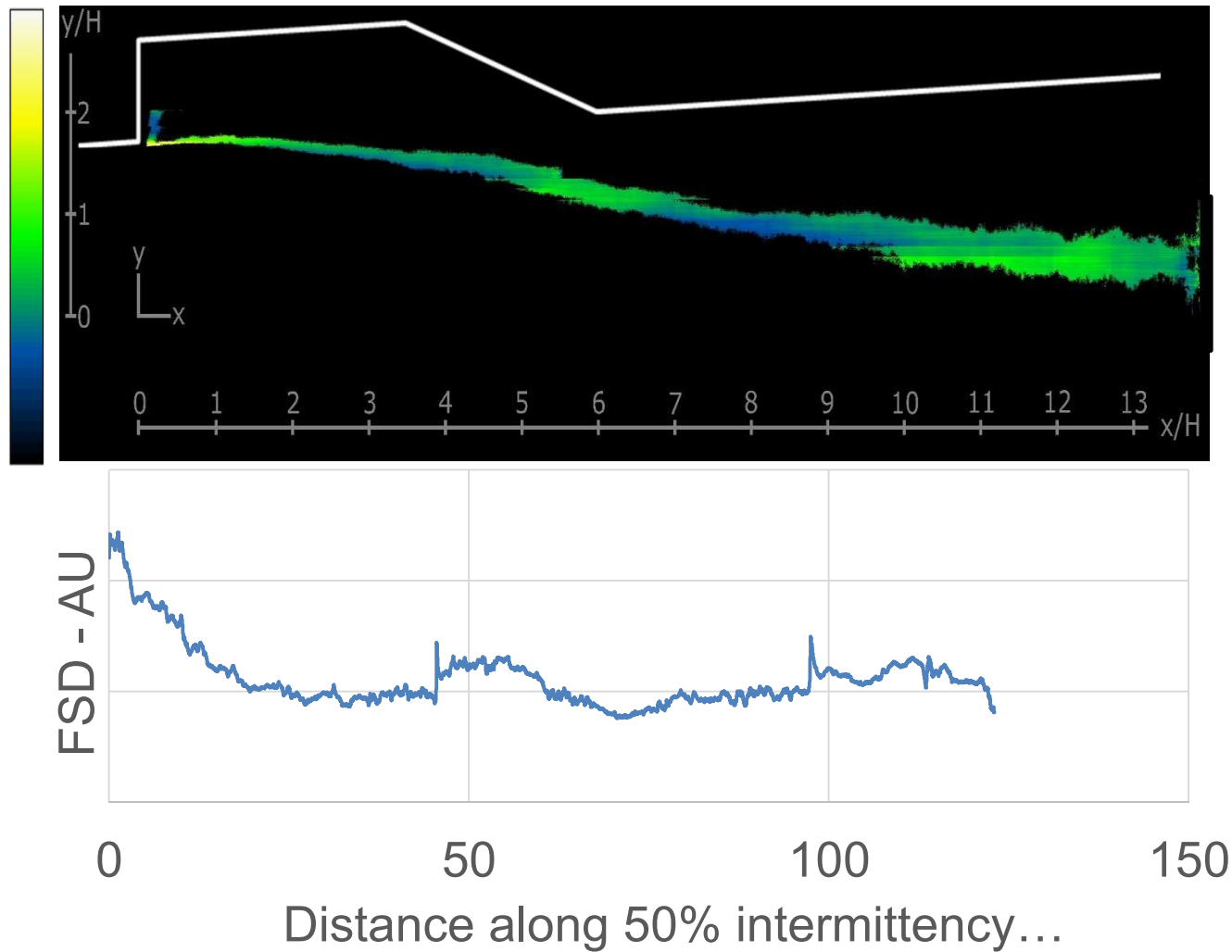
- Flame surface density (FSD):
 - FSD = surface area of the flame per unit volume
 - First step: process image to obtain flame front
 - Threshold method:
 - using ImageJ* iterative threshold approach
- Fractal Dimension:
 - Box counting method

$$N = A \varepsilon^{-D_B}$$

*Ridler, TW & Calvard, S (1978), "Picture thresholding using an iterative selection method", *IEEE Transactions on Systems, Man and Cybernetics* 8: 630-632



FSD Compilation

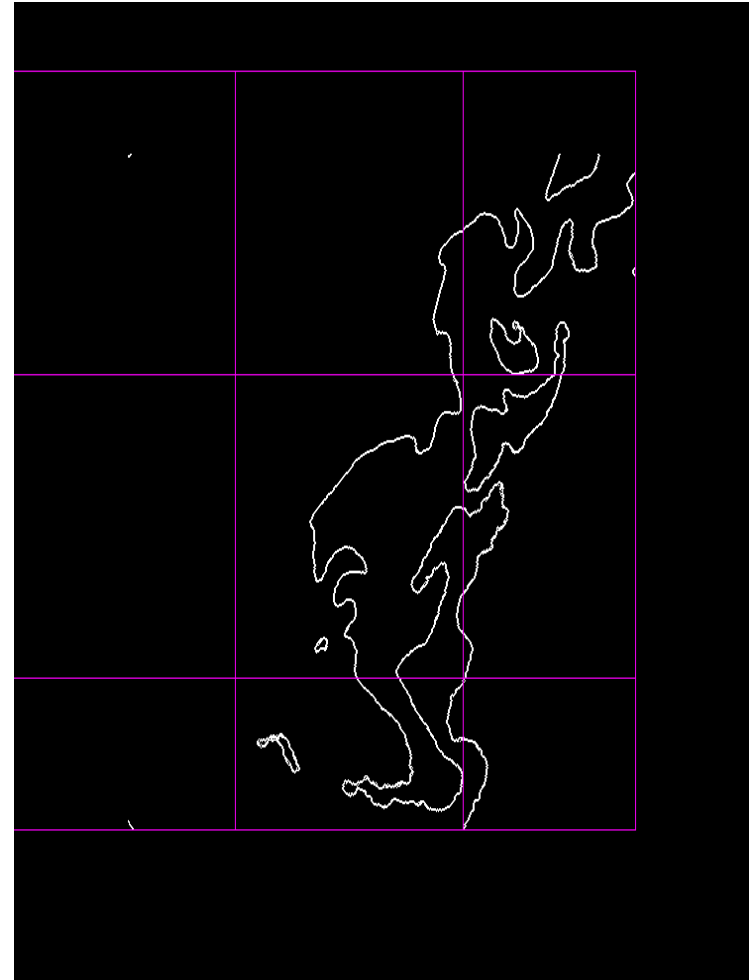
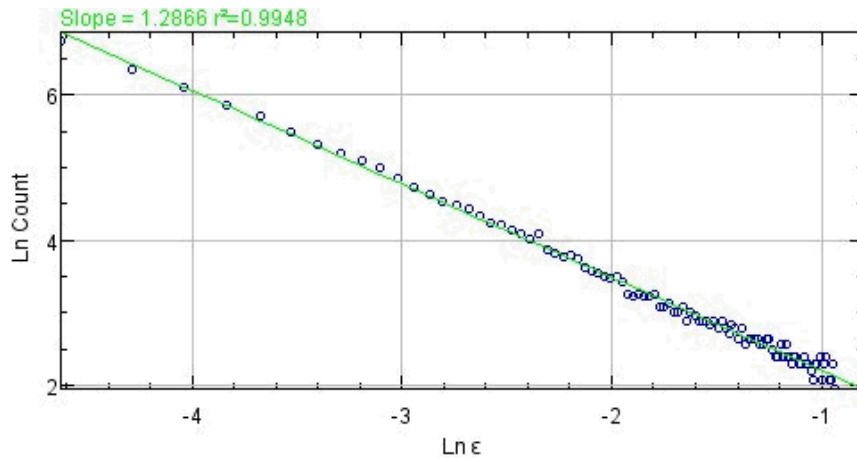


Fractal Dimension – Box Counting Method

- Binarize flame front images
- Overlay grids of various sizes
- Count the number of boxes with flame front pixels N
- Fit logarithmic regression

$$N = A \varepsilon^{-D_B}$$

- Get fractal dimension

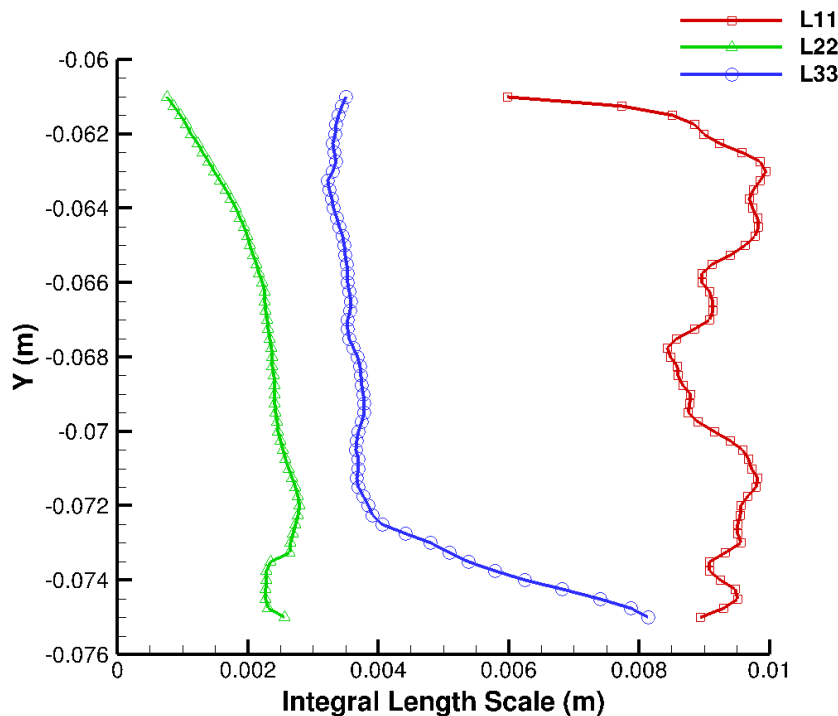


* Karperien, A., *FracLac for ImageJ*. 1999-2013.

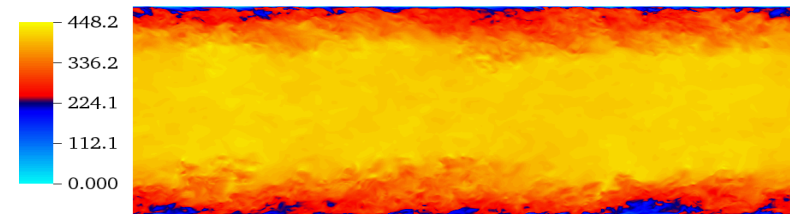
Integral Length Scales from LES

(for $\varphi = 0.43-0.44$)

- Estimated near the leading edge of the insert and consistent with previous PIV measurements ($l_{11}=16$ mm and $l_{22}=4$ mm)
- But shows severe anisotropy!



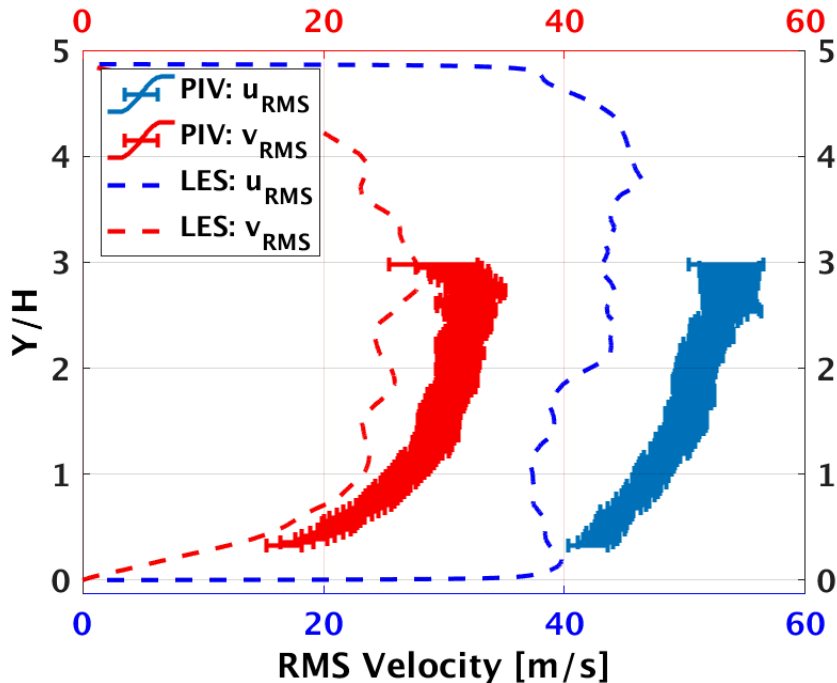
- Can complicate the generation of inflow velocity data for DNS?



Previously generated
turbulent feed from DNS
channel flow

DNS Boundary Conditions

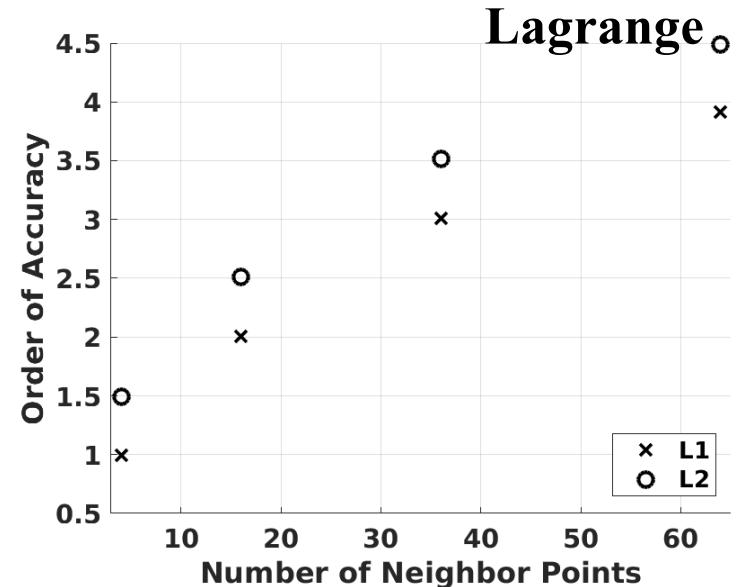
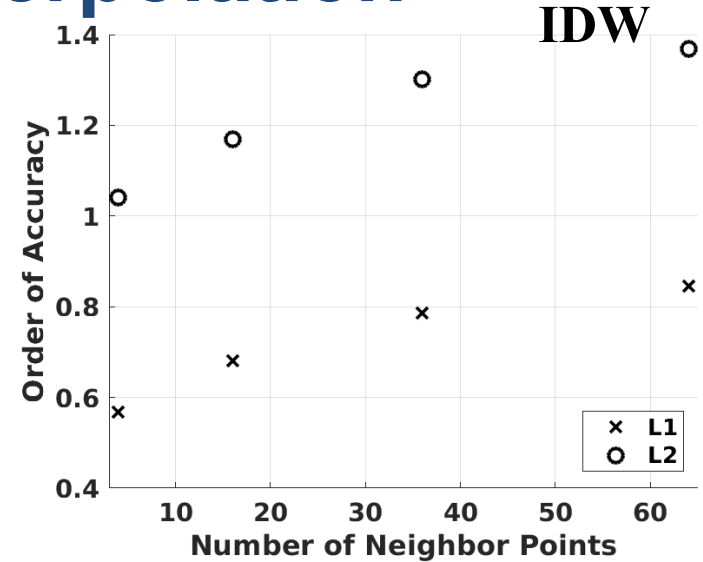
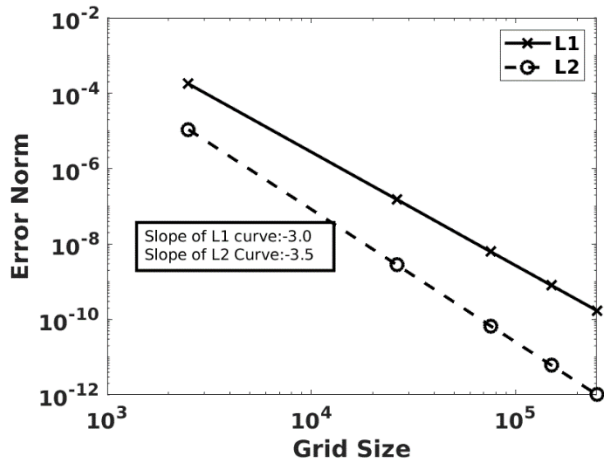
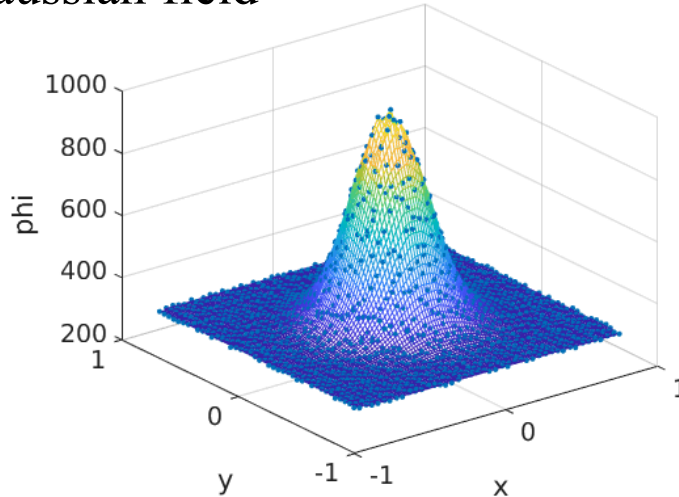
- New approach: generate synthetic turbulence
- Goal: match LES/PIV RMS profiles



- Method:
 1. Generate isotropic turbulence for mean turbulence intensity and streamwise integral length scale in aux. simulation
 2. Filter isotropic turbulence to obtain matching u , v RMS profiles
 3. Correct w' to maintain turbulence spectrum

DNS with IBM: Interpolation

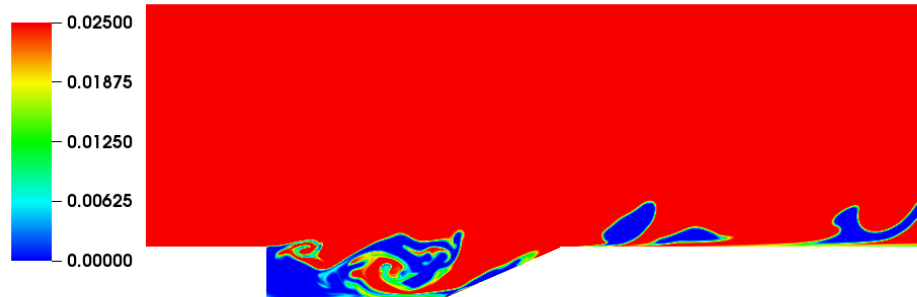
- Interpolation test case: 2D symmetric gaussian field



DNS with Immersed Boundary Method

- DNS with linear close-up ramp simulated in 2D
- Conditions: $M=0.3$, $\phi=0.42$, $T_s = 1125\text{K}$, $p_s = 1.72\text{ atm}$

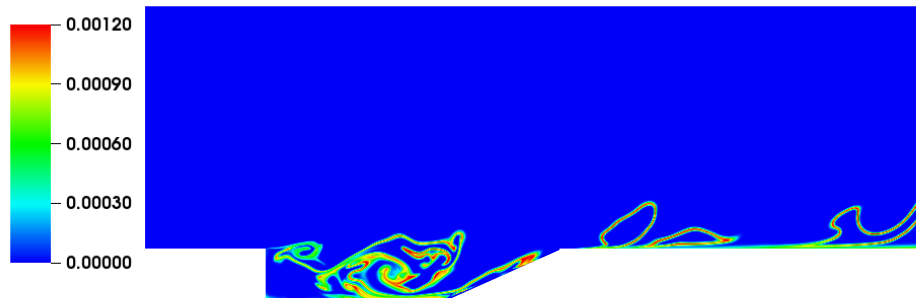
$Y_{\text{C}_2\text{H}_4}$



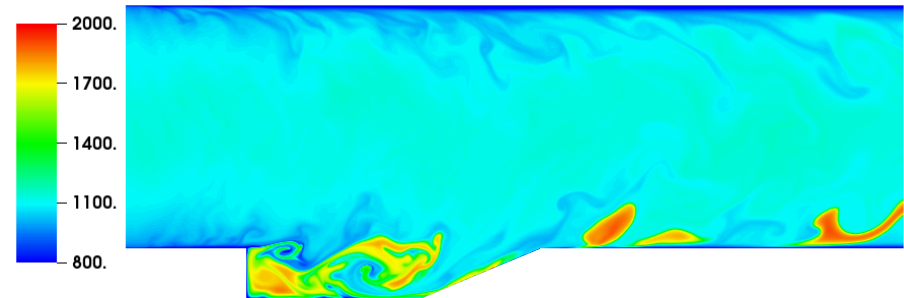
Y_{OH}



$Y_{\text{CH}_2\text{O}}$



$T\text{ [K]}$



Laminar Flame Structure

- Species analysis of cavity case ($T=1125\text{K}$, $p=1.7\text{atm}$, $\phi=0.4$)

