

DIRECT NUMERICAL SIMULATION OF TURBULENCE-CHEMISTRY INTERACTIONS: FUNDAMENTAL SCIENCE TOWARDS PREDICTIVE MODELS

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Acknowledgments

Contributions from:

Ray Grout, Hemanth Kolla, Edward Richardson,
Andrea Gruber, Chun Sang Yoo, Ramanan
Sankaran, Tianfeng Lu

Sponsors:

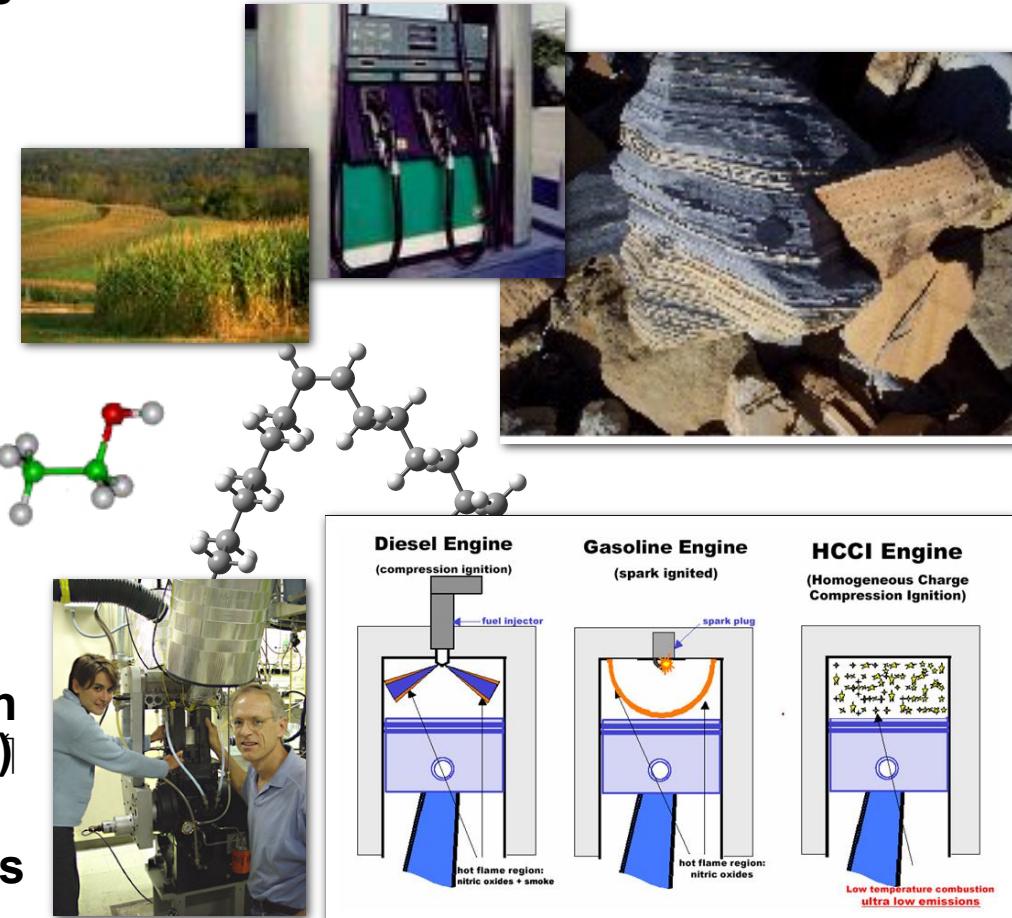
DOE Basic Energy Sciences Division of Chemical
Sciences, Geosciences and Biosciences,
Combustion Energy Frontier Research Center,
Advanced Scientific Computing Research Office

Why combustion? Energy security, climate change, economic competitiveness

- Combustion of fossil fuels accounts for 83% of energy used in U.S.
- Transportation alone accounts for 2/3 of petroleum usage and 1/4 of CO₂ emissions
- National goals to reduce petroleum usage by 25% by 2020 and greenhouse gas emissions by 80% by 2050
- Concurrently new fuels are evolving
- Meeting these goals requires new generation of high efficiency, low emissions combustion systems using diverse future fuel sources
- New scientific understanding to develop predictive, validated multi-scale models to shorten product design cycle

Motivation: Changing World of Fuels and Engines

- Fuel streams are rapidly evolving
 - Heavy hydrocarbons
 - ✓ Oil sands
 - ✓ Oil shale
 - ✓ Coal
 - New renewable fuel sources
 - ✓ Ethanol
 - ✓ Biodiesel
- New engine technologies
 - Direct Injection (DI)
 - Homogeneous Charge Compression Ignition (HCCI)
 - Low-temperature combustion
- New mixed modes of combustion (dilute, high-pressure, low-temp.)
- Sound scientific understanding is necessary to develop predictive, validated multi-scale models!

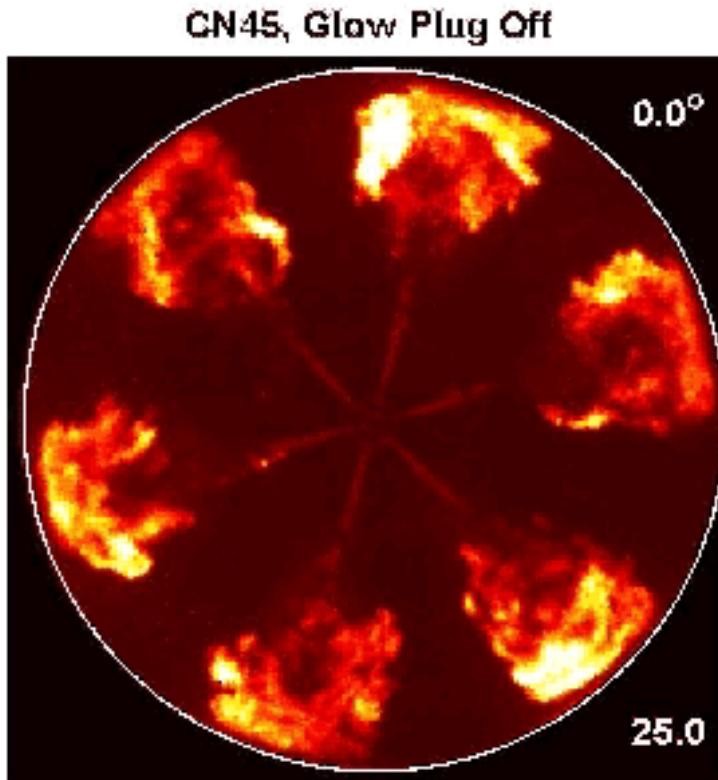


Tailoring fuels to engine design

- *Hundreds* of molecules have been proposed as alternative fuels many from biology.
 - How to assess which are worth pursuing? Not practical to run them all in comprehensive engine tests
 - Full engine experimental campaigns would require manufacturing large amount of each proposed new fuel and fuel blend...
- Many new engine designs in development, not clear which engine to use to test future fuels.
 - Experimentally building/testing each new engine is expensive and slow; fuel-in-engine experiments are relatively expensive and unreliable
 - Fuel needs to work over broad range (T, P, Composition)
 - Hard to experimentally test over the whole range of conditions
- Ability to *predict* behavior of new fuels at many conditions, and in proposed engine designs, would be extremely valuable!

Anecdote from Professor Bill Green, MIT

IC Engine Combustion Is A Complex, Multi-physics, Multi-scale Problem



Diesel Engine Autoignition, Soot Incandescence
Chuck Mueller, Sandia National Laboratories

Stiffness : wide range of length and time scales

- In-cylinder geometry (cm)
- Turbulence-chemistry (mm)
- Soot inception (nanometer)

Chemical complexity

- large number of species and reactions (100's of species, thousands of reactions)

Multi-Physics complexity

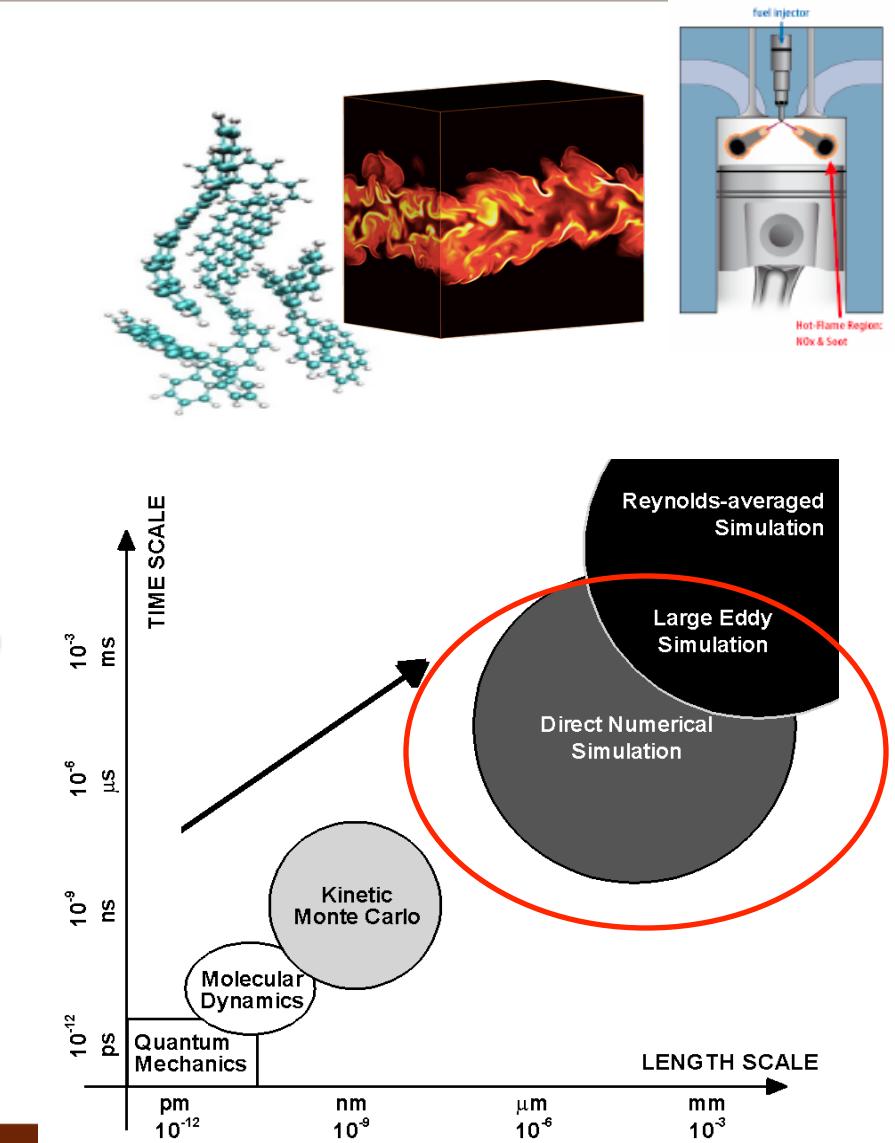
- multiphase (liquid spray, gas phase, soot, surface)
- thermal radiation
- acoustics ...
- All these are tightly coupled

Multi-scale Modeling of Combustion Processes

- Multi-scale modeling describes combustion processes, from quantum scales up to device-level, continuum scales

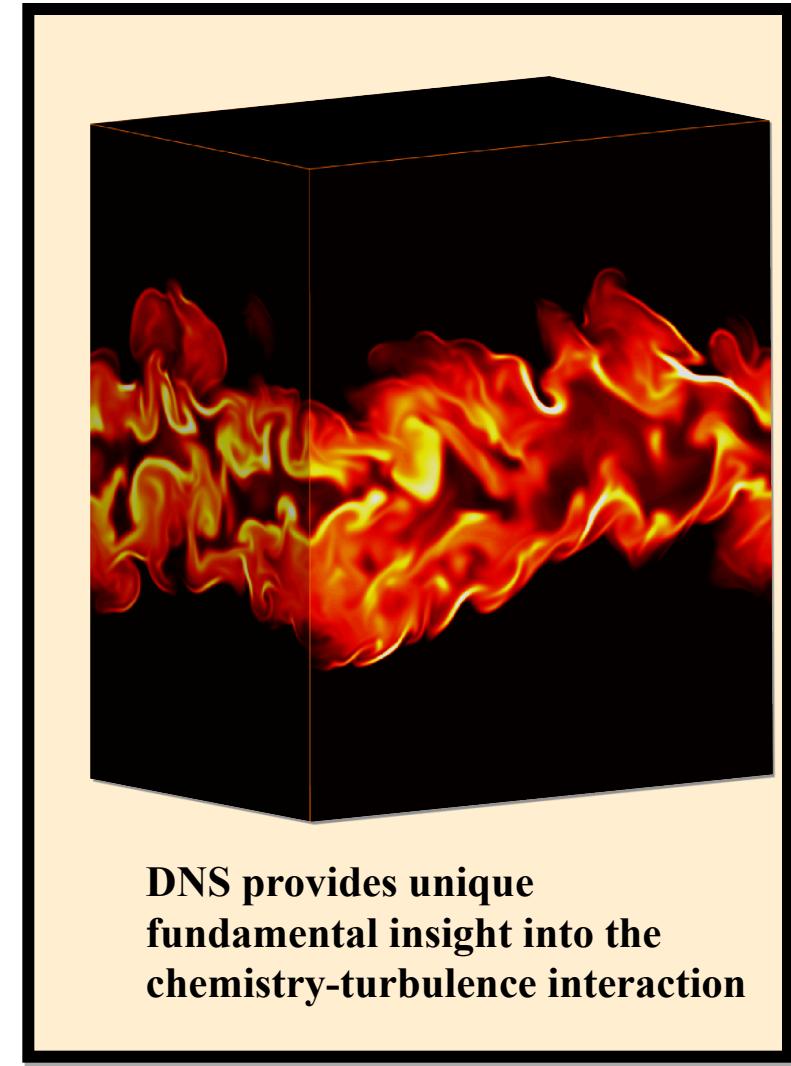
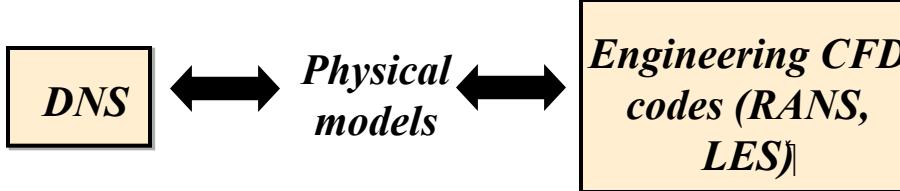
- **Multi-scale Strategy:**

Use petascale computing power to perform direct simulation at the atomistic and fine-continuum scales (~4 decades), and develop new parameterizations that will enable bootstrapping information upscale



Direct Numerical Simulation (DNS) – Sandia S3D

- Used to perform first-principles-based DNS of reacting flows
- Solves compressible reacting Navier-Stokes equations
- High-fidelity numerical methods
- Detailed reaction kinetics and molecular transport models
- Multi-physics: sprays, radiation and soot
- Ported to all major platforms, scales well on petascale machines
- Particle tracking capability



Chemistry-Turbulence Interactions

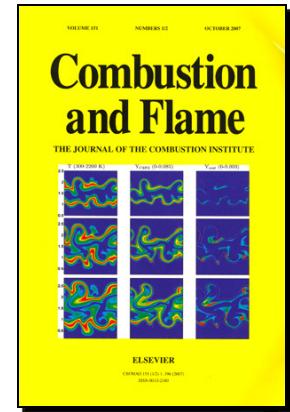
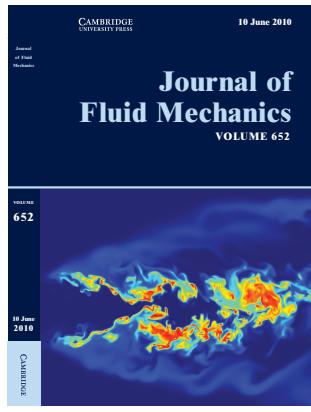
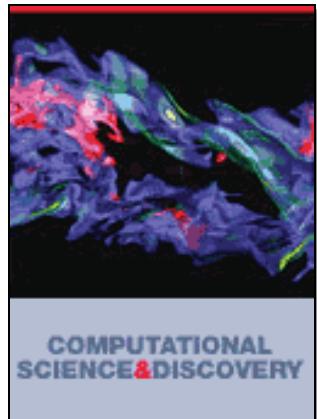
- Turbulence entrains, advects, strains and wrinkles a flame creating more area for burning
- Through turbulence cascade eventually reactants are molecularly mixed
- Chemical reactions are enhanced with mixing to a limit – extinction - and create heat release
- Heat release, dilatation reduce turbulence intensity through density, and property changes
- Need Capability computing: $N_{\text{grids}} = Re^{9/4}$

Role of DNS

- Glean fundamental insight into ‘turbulence-chemistry’ interactions in canonical configurations relevant to transportation and power generation
- Validation data for development of RANS and LES subgrid mixing and combustion models used in engineering CFD
- Validation of chemical mechanisms over relevant aero thermochemical conditions (wide range of T, P, compositions)



Combustion DNS Enabled by Large Computer Allocations



Preparing for the Future: Hybrid Multi-Core Architectures (Titan 10-20 Pflop)

OLCF-3 Application Readiness:

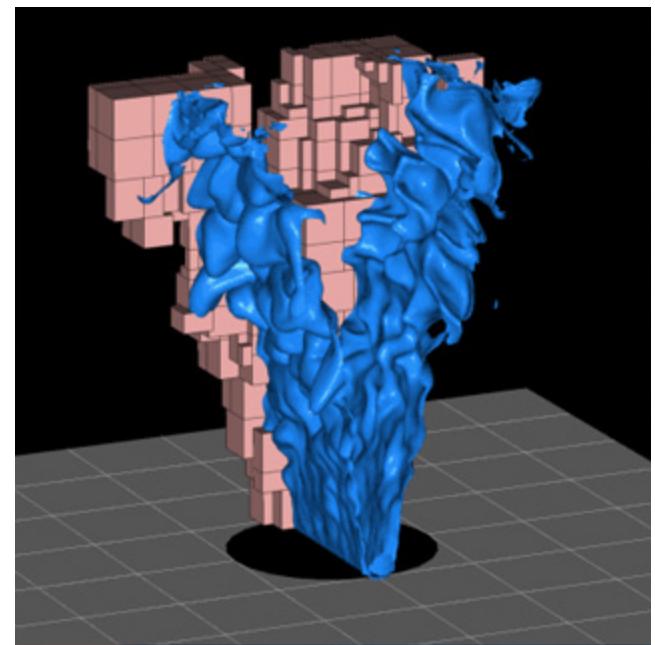
Ray Grout (NREL), John Levesque (Cray),
Ramanan Sankaran (ORNL), Cliff Woolley and Stan Posey (nVidia) refactored S3D in preparation for 10-20 Pflop multi-core hybrid architectures like Titan

Stay tuned for Ray's talk!

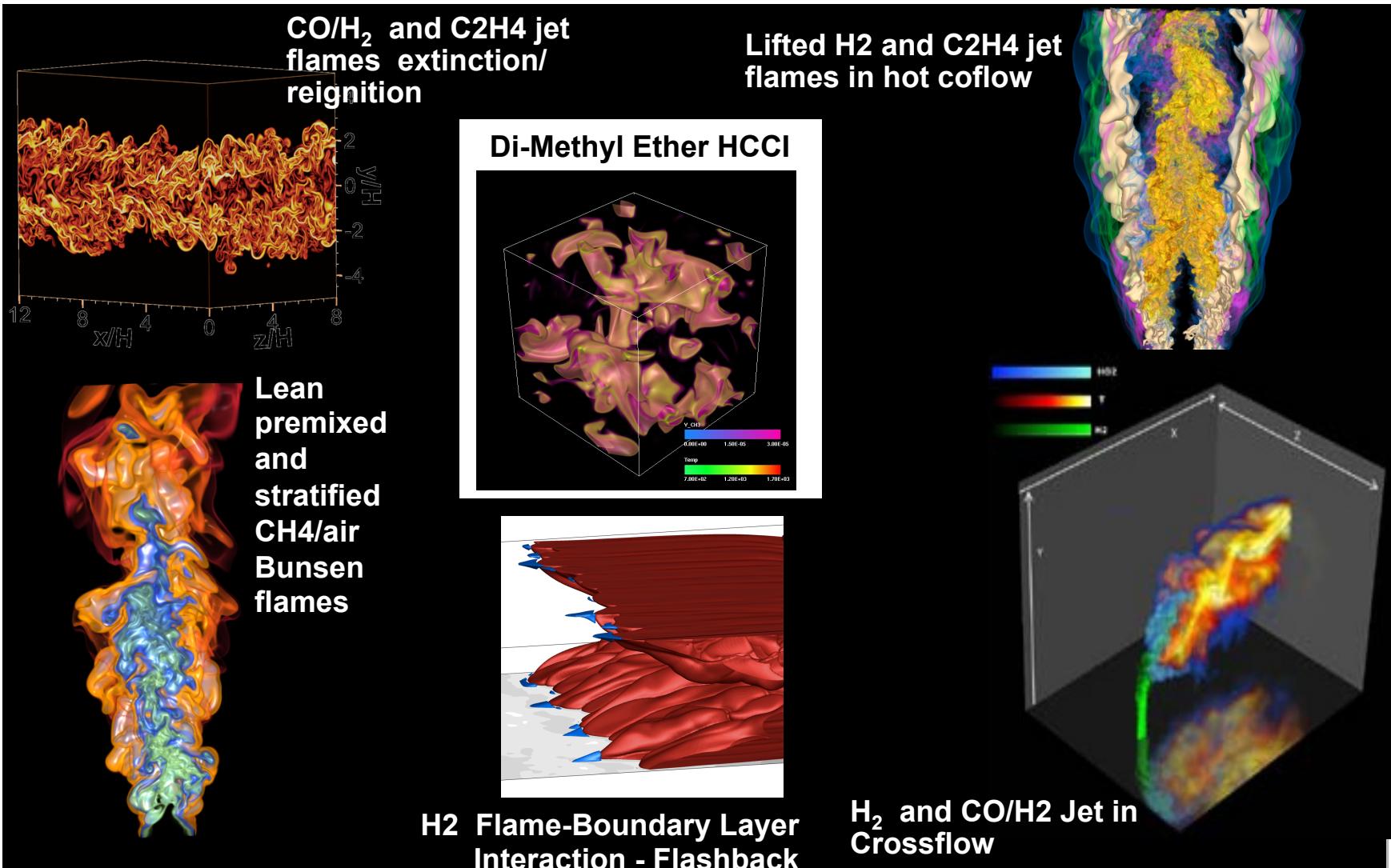
Exascale Combustion Co-Design Center

Through co-design combustion science requirements influence computer architecture design and technology constraints inform design of algorithms and software

- Compressible and low-Mach high-order adaptive mesh refinement
- In situ uncertainty quantification (adjoint sensitivities and polynomial chaos expansion)
- In situ topological analytics and visualization



DNS Benchmarks for Model Development and Validation



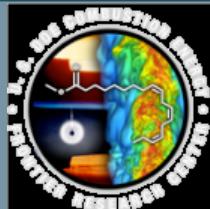
Role of DNS – Case Studies

- Homogeneous Charge Compression Ignition (HCCI) Combustion
- Turbulent Jet Flames in Heated Co-Flow
- Turbulent Jet Flames in Cross-Flow

Role of DNS – Case Studies

- **Homogeneous Charge Compression Ignition (HCCI) Combustion**
- Turbulent Jet Flames in Heated Co-Flow
- Turbulent Jet Flames in Cross-Flow

DNS of Autoignition in Stratified Di-Methyl Ether (DME)/Air Turbulent Mixtures



Gaurav Bansal and Jackie Chen

Combustion Research Facility

Sandia National Laboratories, USA

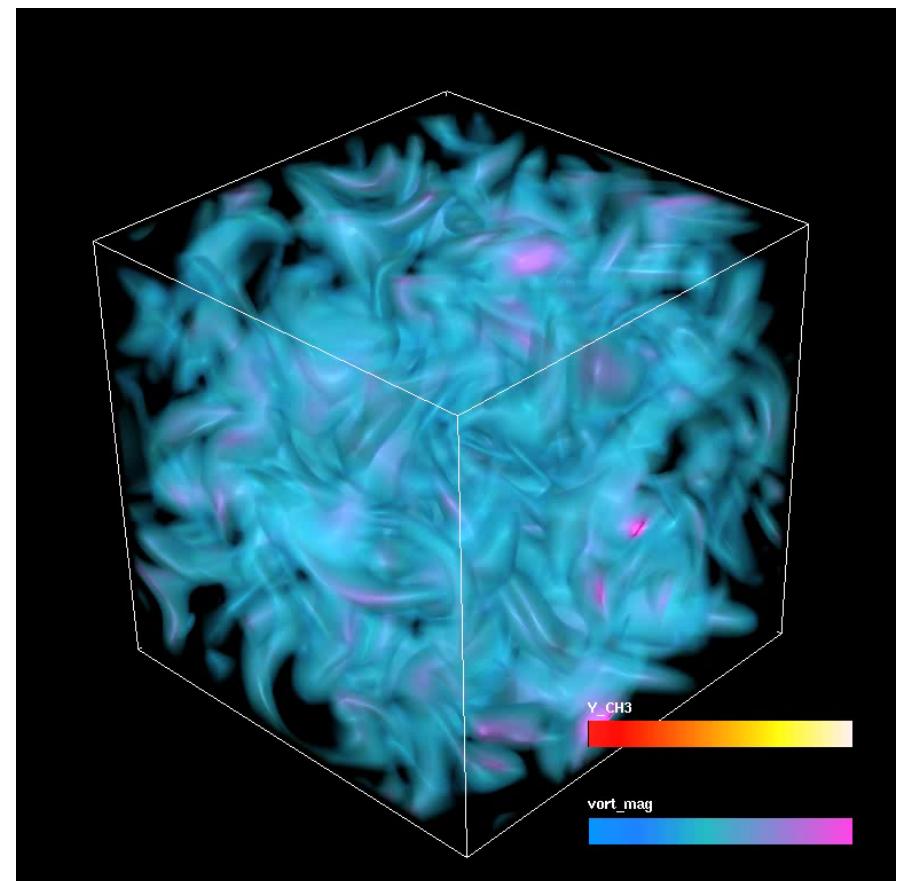
Tianfeng Lu & Zhaoyu Luo

University of Connecticut, USA

Numerical Combustion Meeting, Corfu

Greece, 2011

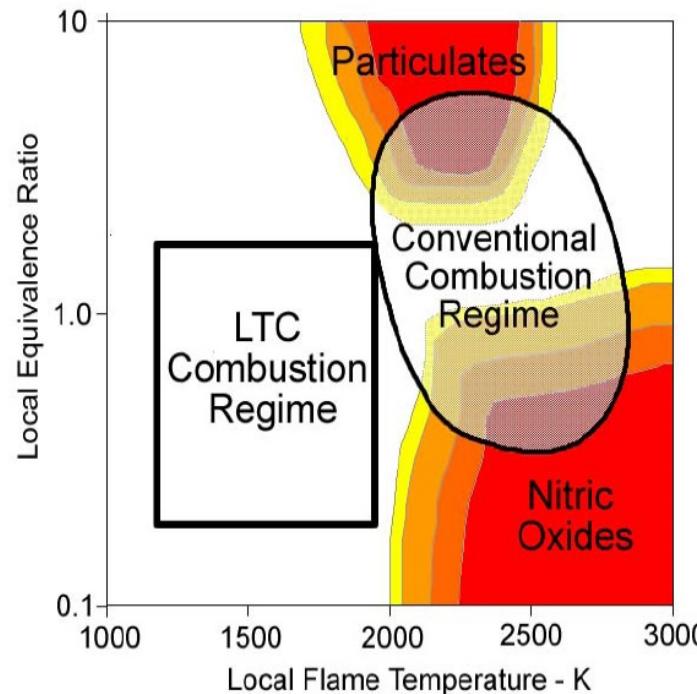
In prep. for Combust. Flame, 2012



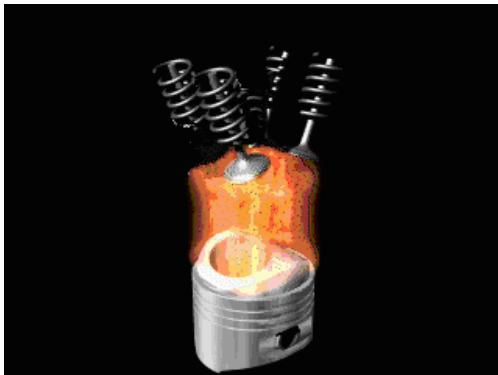
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Homogeneous Charge Compression Ignition (HCCI) Engines

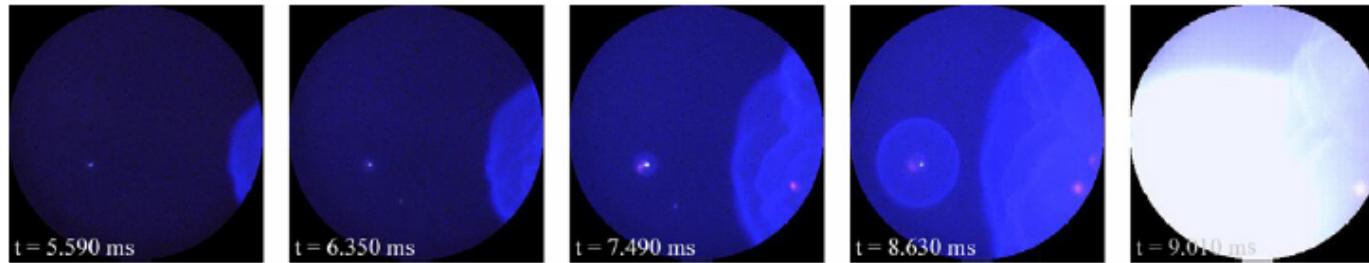


- Potential for high diesel-like efficiencies but low soot and NO_x emissions
- Fuel-lean and at low temperatures – no flame, spontaneous autoignition
- Hard to control ignition timing, sensitive to fuel chemistry, need to moderate burn rate (high load)
- Better understand ignition chemistry of fuel blends and oxygenated hydrocarbon molecules in biomass derived fuels



Optimum combined fuel chemistry and mixing to moderate the rate of combustion in HCCI engines

- Inhomogeneities (thermal or composition) lead to sequential ignition front propagation down a temperature gradient - combustion modes ranging from homogeneous explosion to propagating flames
- New modes operate far from equilibrium with highly transient intermittent ignition occurring at multiple sites
- Low pre-ignition temperatures, strong finite-rate kinetic effects due to competition between mixing and chemistry
- Strong sensitivities to fuel chemistry and mixing provide multiple control options (e.g. combustion retard, multiple fuel injection)
- Better understand and predict behavior of alternative fuels in HCCI engines



Optical engine experiments by Walton et al. show front-like propagation

Mixture inhomogeneities reduce peak heat release rates and pressure rise rates – hot spots preferred ignition spots – deflagration waves or spontaneous ignition?

DNS of DME HCCI Autoignition

Turbulence and scalars initialized using an energy spectrum

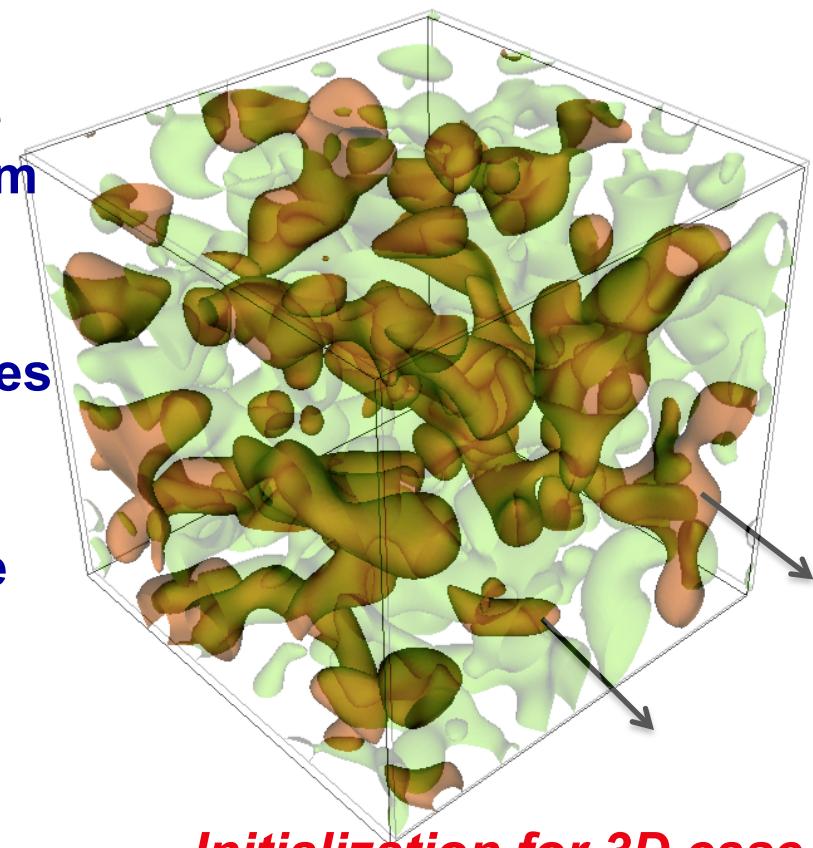
Initial turbulence integral time-scale and scalar RMS values – guided from practical engine experiments

Reduced DME chemistry – 30 species

Initially homogeneous composition ($\phi = 0.3$) with Gaussian temperature distribution, $T' = 25K$

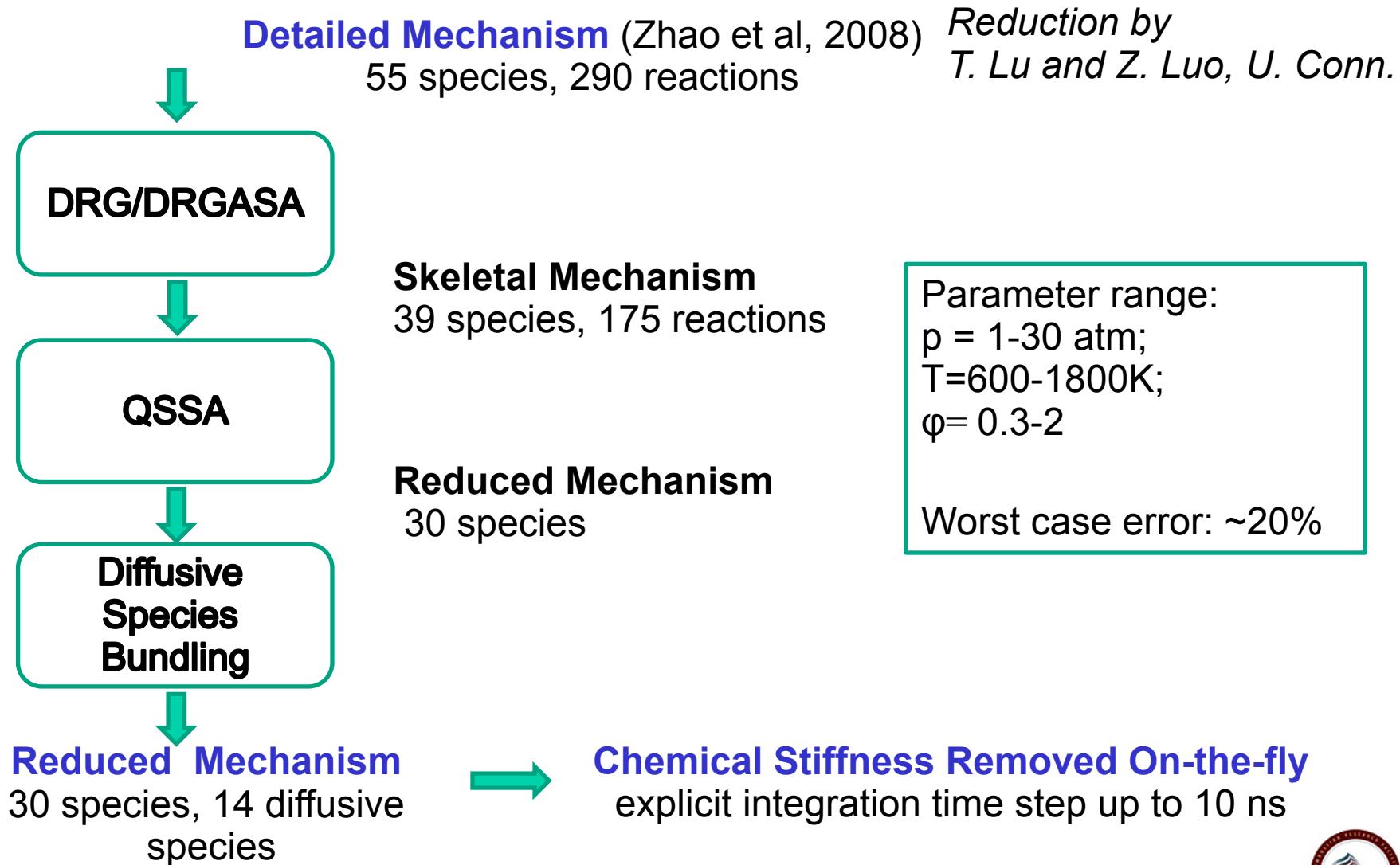
Mixture averaged transport

Isentropic compression simulates HCCI engine operation from 36 CAD to TDC



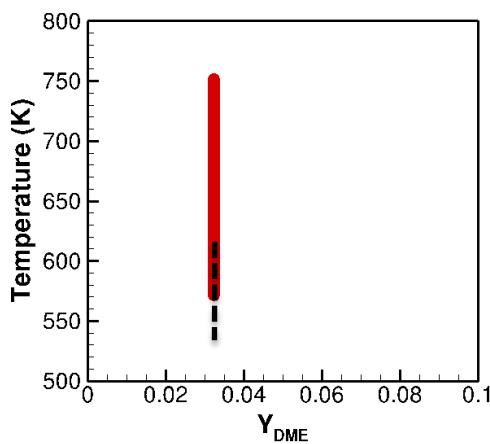
Initialization for 3D case

DME Chemistry Reduction Procedure

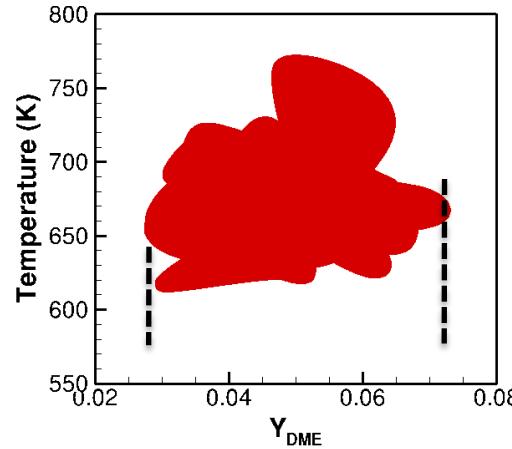


Three-stage Ignition in DME/Air Mixtures with Thermal and Composition Stratification

Initial Conditions



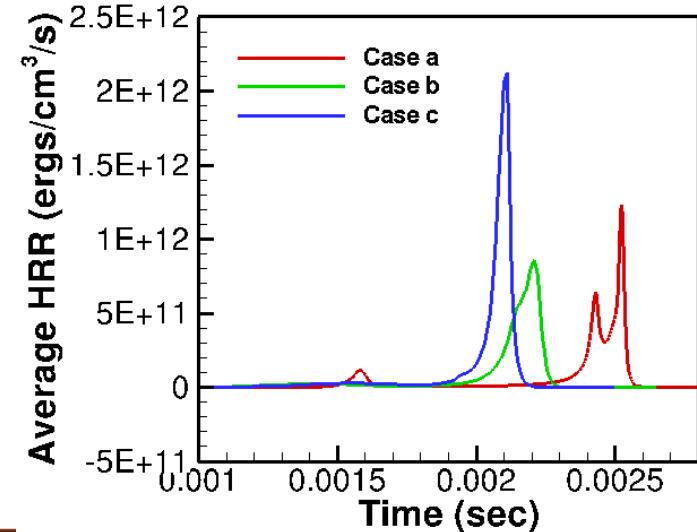
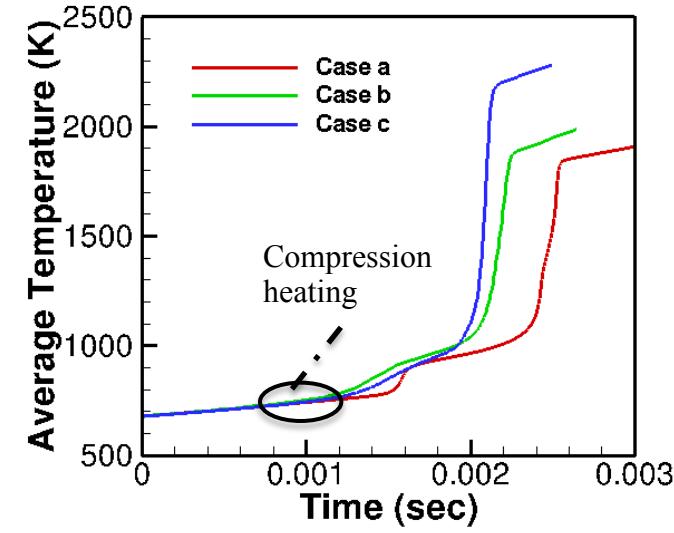
Case b



Case c
(with 70% EGR)

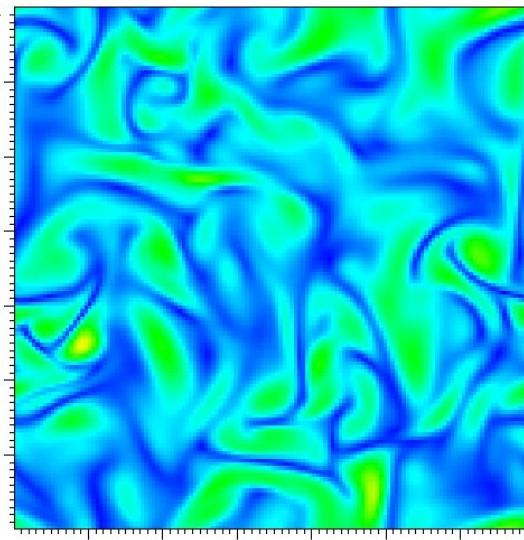
Initial mean temperature 678K, pressure = 10.8 atm
Compression ratio of 18:1, rpm=1200

- I. LTC ignition, $\text{CH}_3\text{OCH}_2\text{O}_2$ (low T)
- II. H_2O_2 dissociation (intermediate T)
- III. $\text{H} + \text{O}_2 = \text{OH} + \text{O}$ (high T)

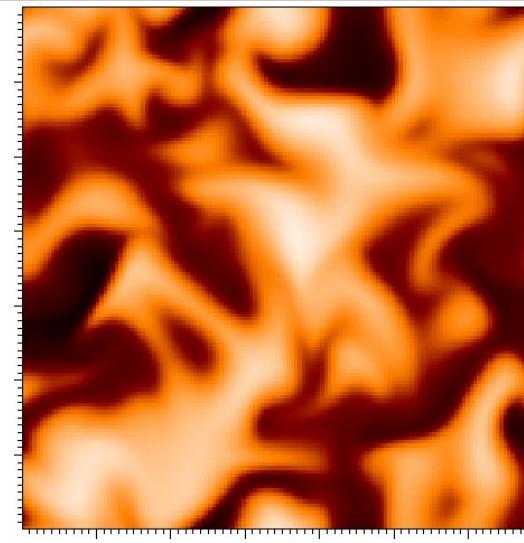


Existence of highly wrinkled thin “cool flame” fronts – first ignition stage

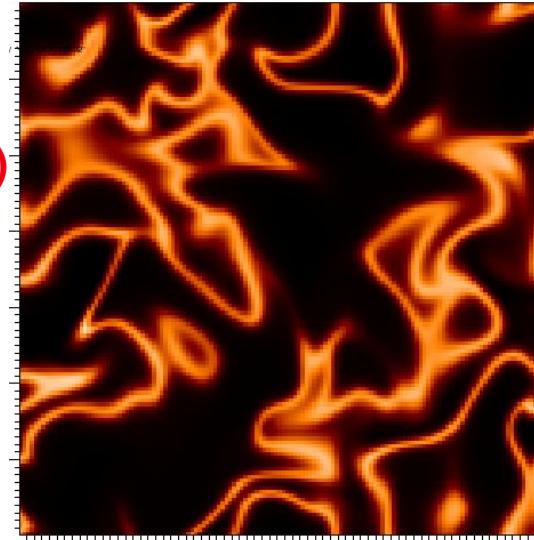
Vorticity



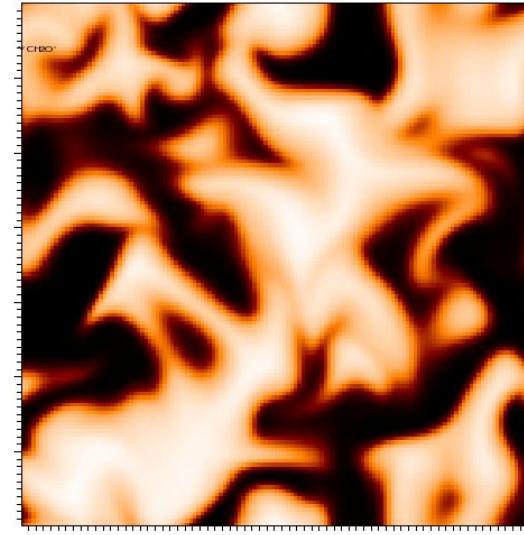
Temp



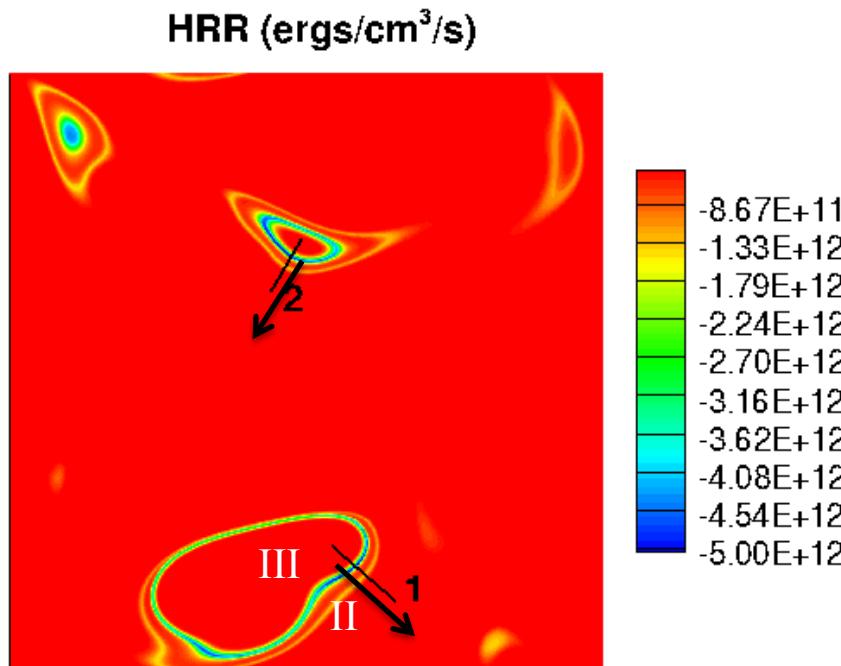
$Y_{CH3OCH2O2}$
(Key intermediate)



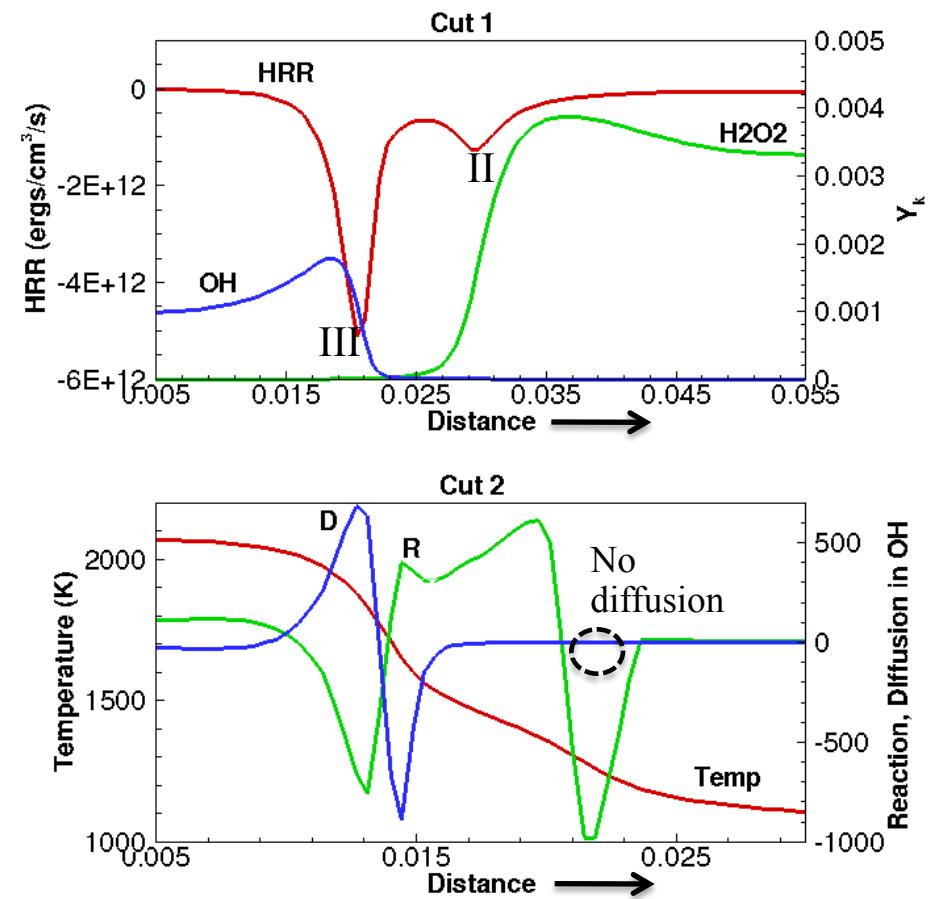
Y_{CH2O}



Simultaneous Existence of Flames and Spontaneous Ignition

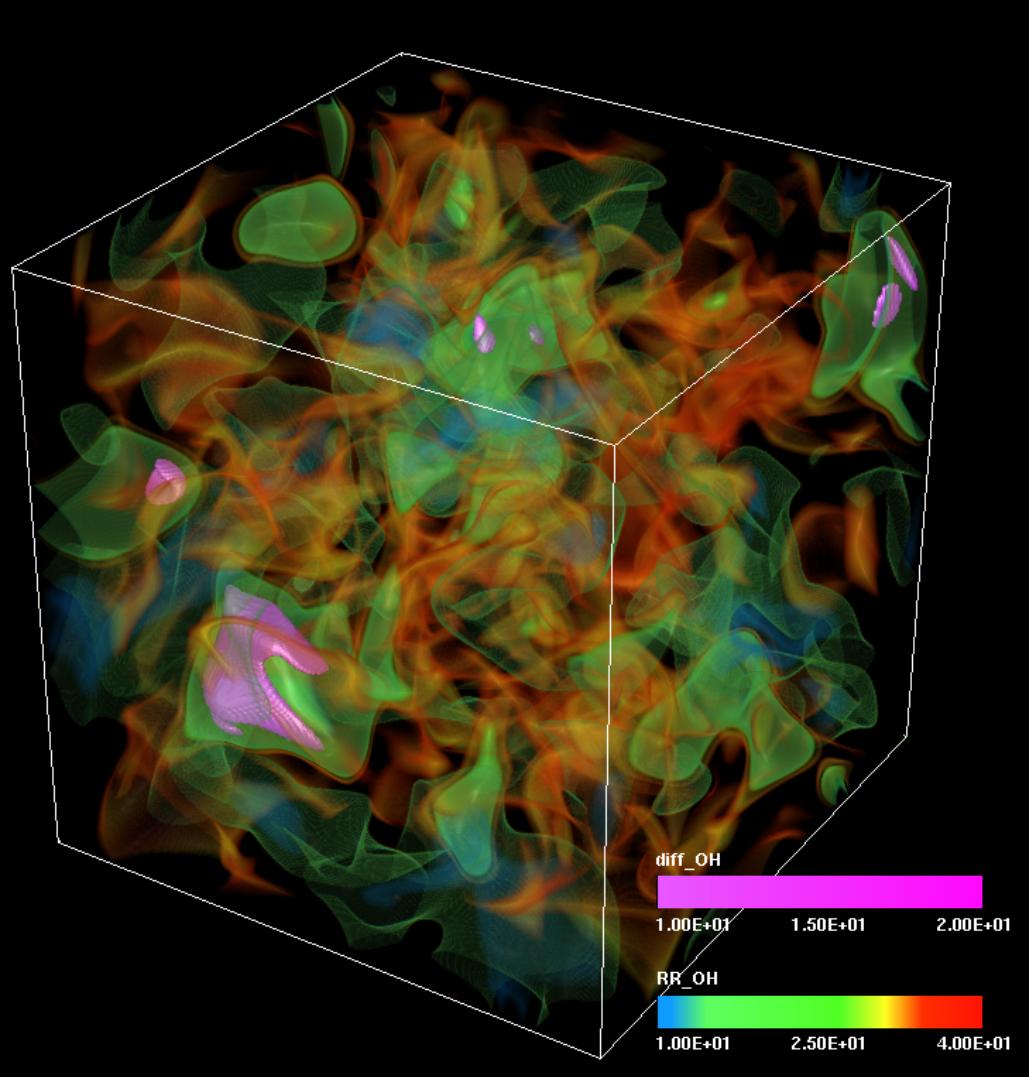


A twin-ring structure of heat release



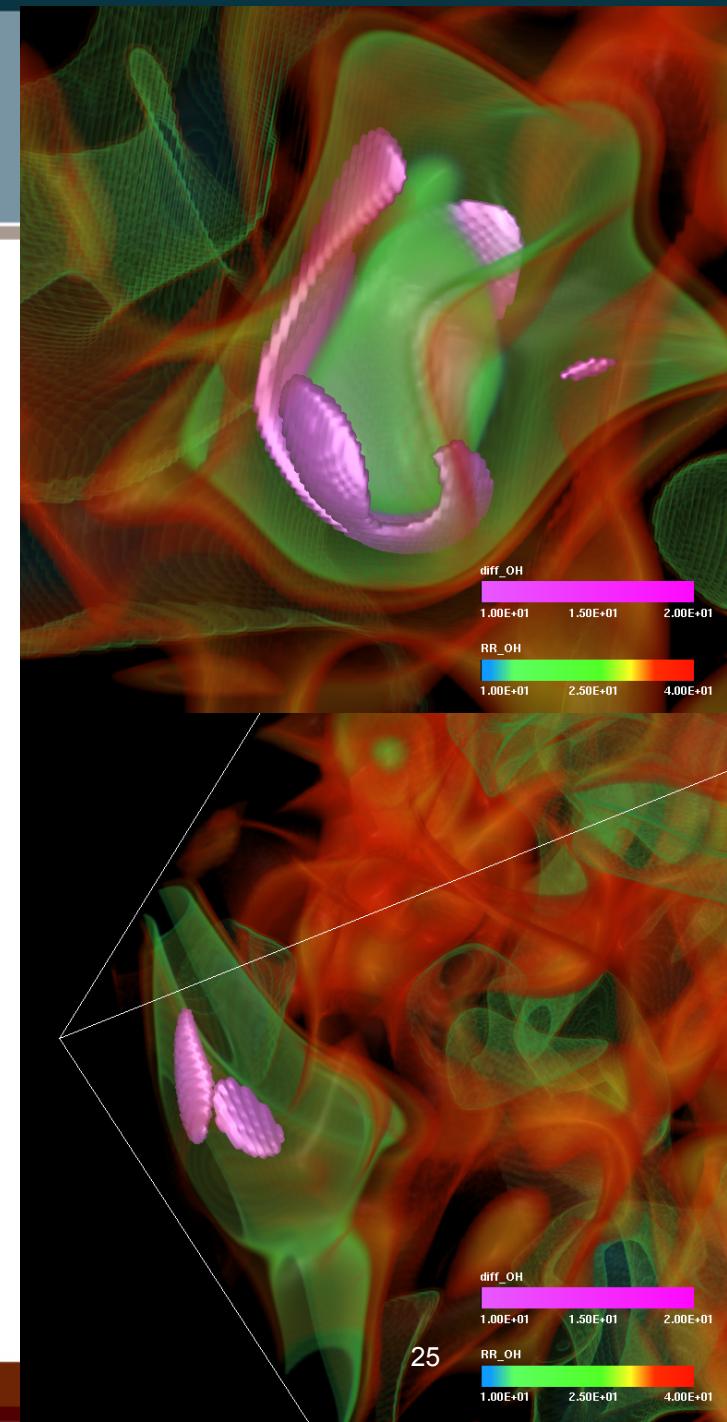
Close proximity of IInd and IIIrd stage waves – inter-diffusion of heat and radicals
IInd stage is chemistry driven spontaneous front; IIIrd stage is a deflagration wave

Reaction-Diffusion Structure



Time = 2.1500 msec

TRANSPORTATION ENERGY CENTER



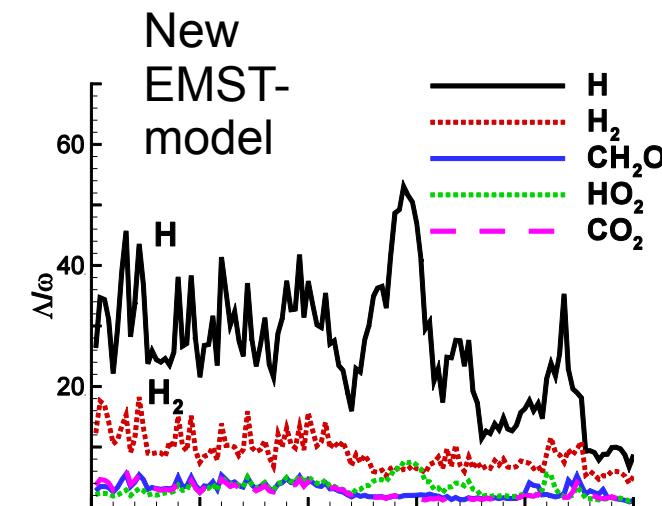
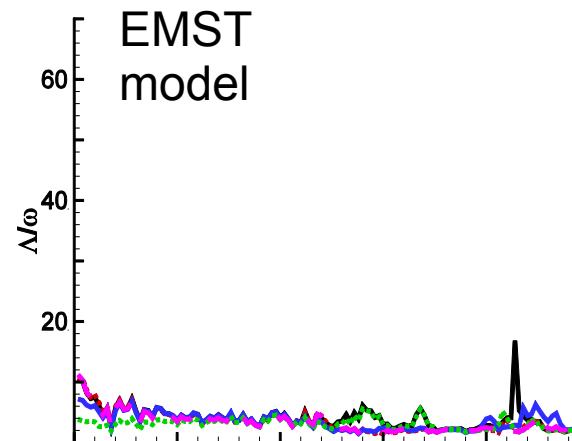
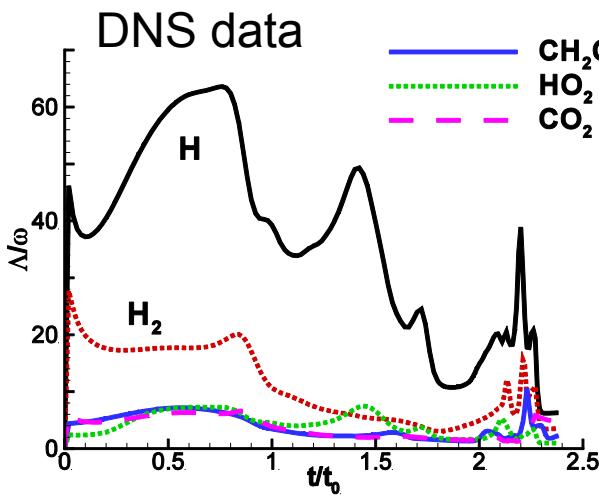
Transported PDF Modeling of Molecular Mixing in Flames With Differential Diffusion

- Differential diffusion of species provides a mechanism for different molecules to diffuse at different speeds – strongly influencing flame dynamics, pollution, and radiation.
- DNS is currently the ONLY tool that gives resolved 3D information on differential diffusion physics in turbulent flow.
- DNS data are providing unprecedented opportunities to validate and refine predictive models.
- Transported PDF methods handle mixed mode combustion – provides exact closure for chemical source terms, but multi-scalar molecular mixing requires modeling in both RANS and as a subgrid LES model
- Can we model differential diffusion in a PDF mixing model that satisfies conservation of means, localness, and realizability?

PDF modeling of molecular mixing in flames with differential diffusion

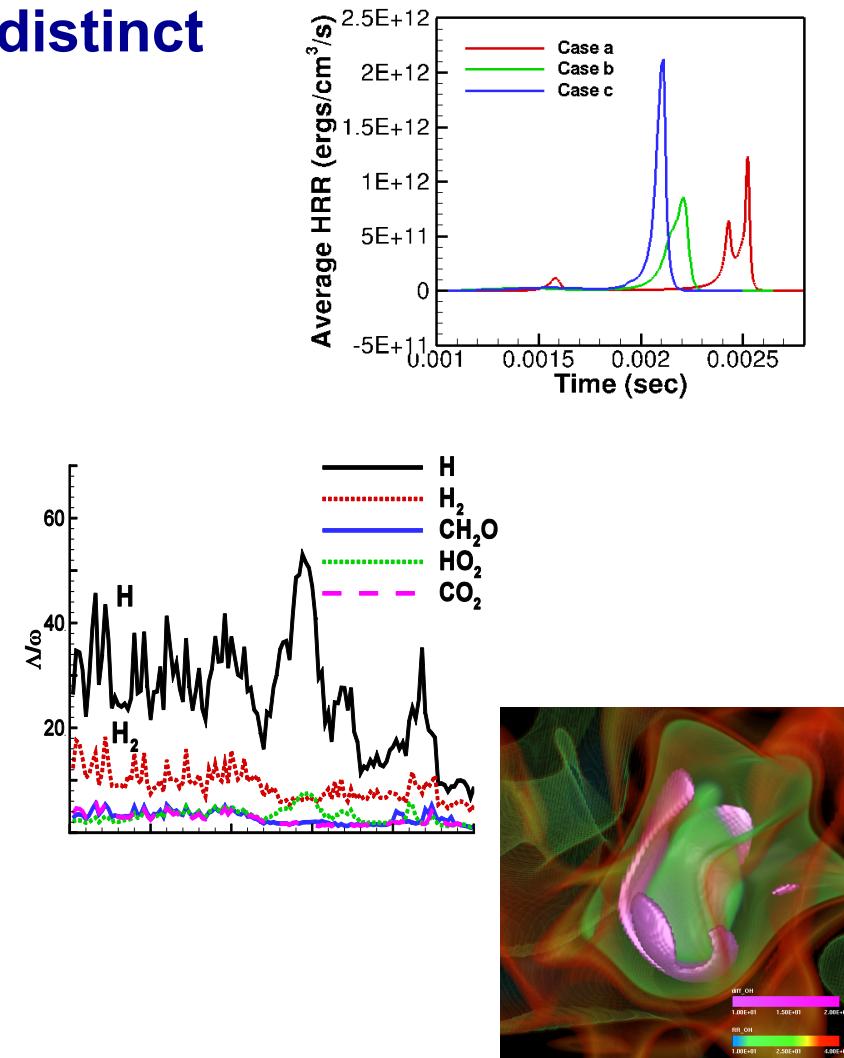
- The DNS data reveal individual species mixing at vastly different rates – due to species diffusivities and flame structure.
- Predictions of the state-of-the-art EMST model: Accounts for flame structure but unable to account for differential diffusion.
- New PDF modelling developed by Richardson and Chen (*Combustion and Flame* 2012) includes species diffusivities in a rigorous manner and correctly predicts the physics observed in the DNS.

Variation of normalised species mixing rates versus time:



Summary of DME HCCI DNS and Modeling

- **DME autoignition occurs in three distinct chemical stages**
- **2nd and 3rd stage can occur in close physical proximity**
- Due to strong reaction generated gradients –scalar dissipation due to reaction
- Multi-scalar mixing models treating localness and differential diffusion (EMST-DD)
- 2nd stage is predominantly spontaneous ignition front; 3rd stage is predominantly premixed deflagration

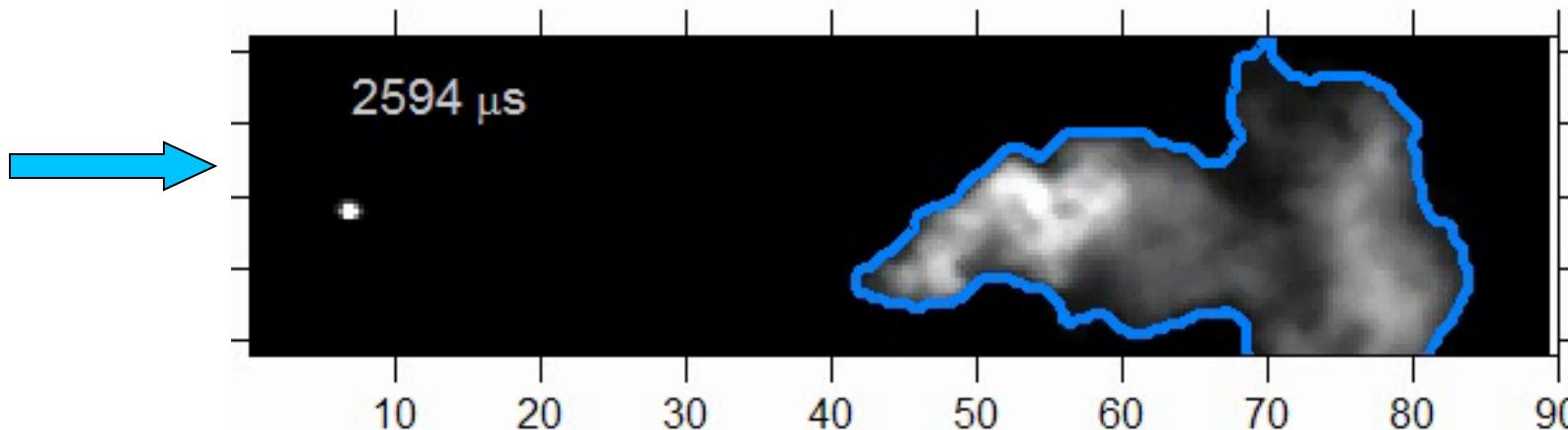


Role of DNS – Case Studies

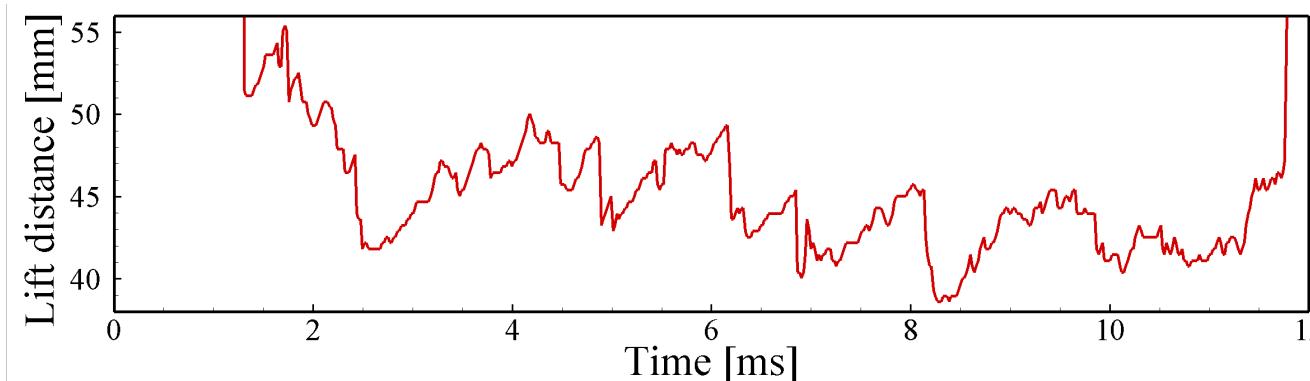
- Homogeneous Charge Compression Ignition (HCCI) Combustion
- **Turbulent Jet Flames in Heated Co-Flow**
- Turbulent Jet Flames in Cross-Flow

Motivation: Understanding Stabilization of Lifted Flames in Heated Coflow

What is the role of ignition in lifted flame stabilization?



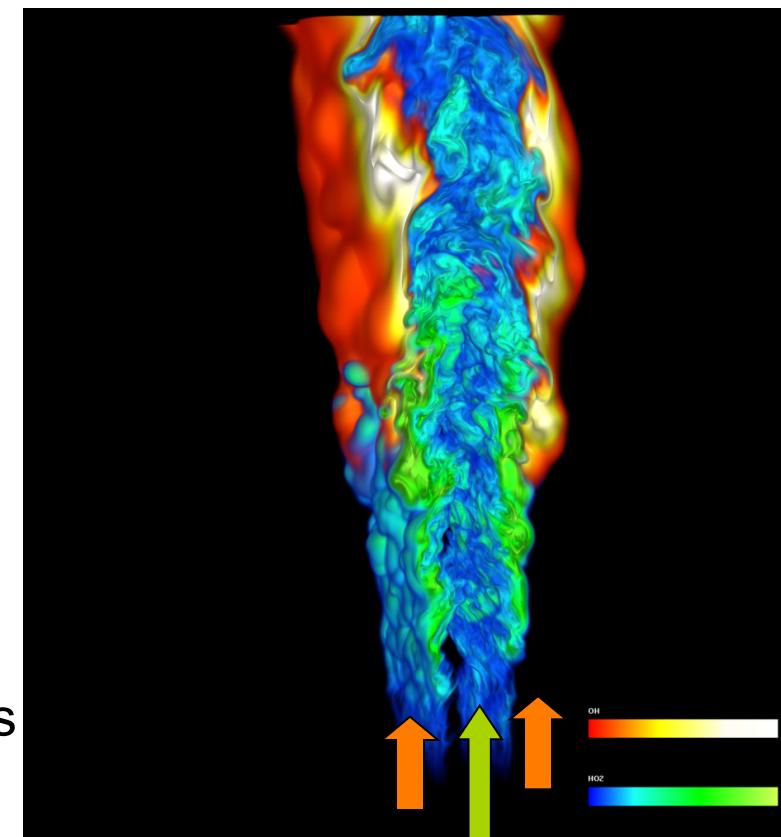
Chemiluminescence from diesel lift-off stabilization for #2 diesel, ambient 21% O₂, 850K, 35 bar courtesy of Lyle Pickett, SNL



DNS of Lifted Ethylene-air Jet Flame in a Heated Coflow

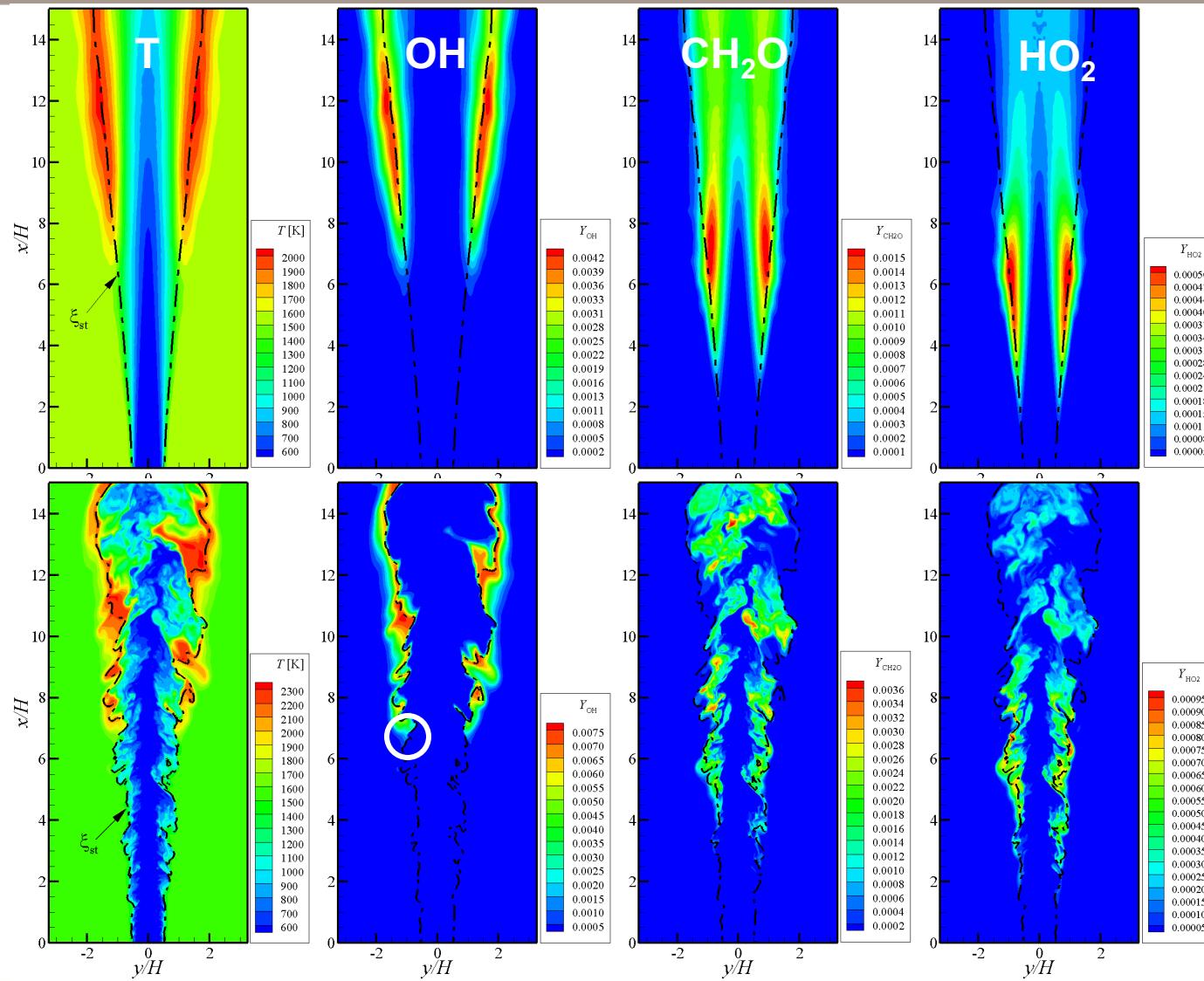
- 3D slot burner configuration:
 - $L_x \times L_y \times L_z = 30 \times 40 \times 6 \text{ mm}^3$ with
 - 1.28 billion grid points
 - High fuel jet velocity (204m/s); coflow velocity (20m/s)
 - Nozzle size for fuel jet, $H = 2.0\text{mm}$
 - $\text{Re}_{\text{jet}} = 10,000$
 - Cold fuel jet ($18\% \text{ C}_2\text{H}_4 + 82\% \text{ N}_2$) at 550K, $\eta_{\text{st}} \approx 0.27$
 - Detailed C_2H_4 /air chemistry, 22 species 18 global reactions, 201 steps
 - Hot coflow air at 1,550K

C. S. Yoo, et al. *Proc. Comb. Inst.* 2011

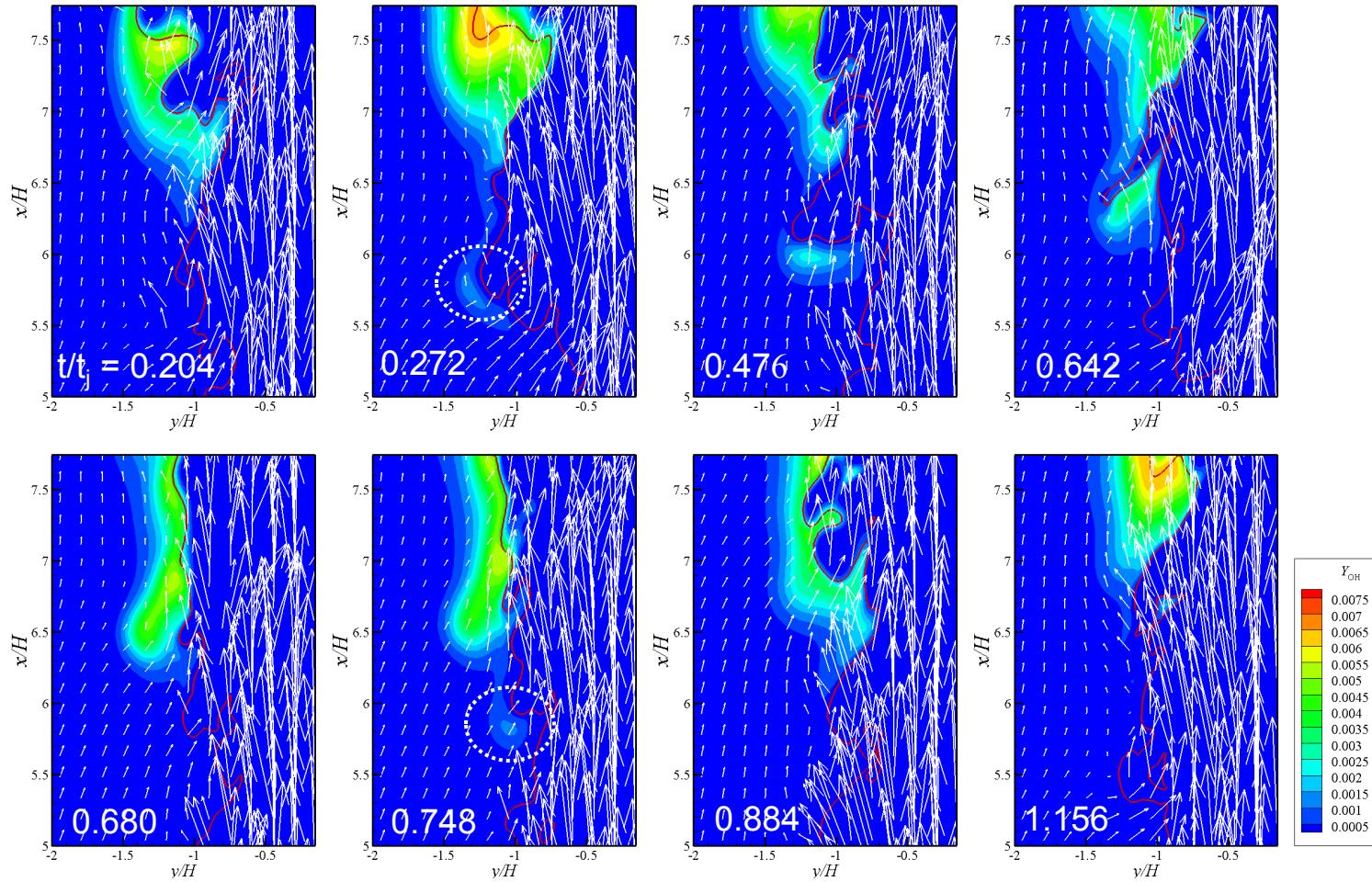


Ethylene-air lifted jet flame at $\text{Re}=10000$

Favre Mean and Instantaneous Temperature and Species Mass Fractions (OH, CH₂O, HO₂)

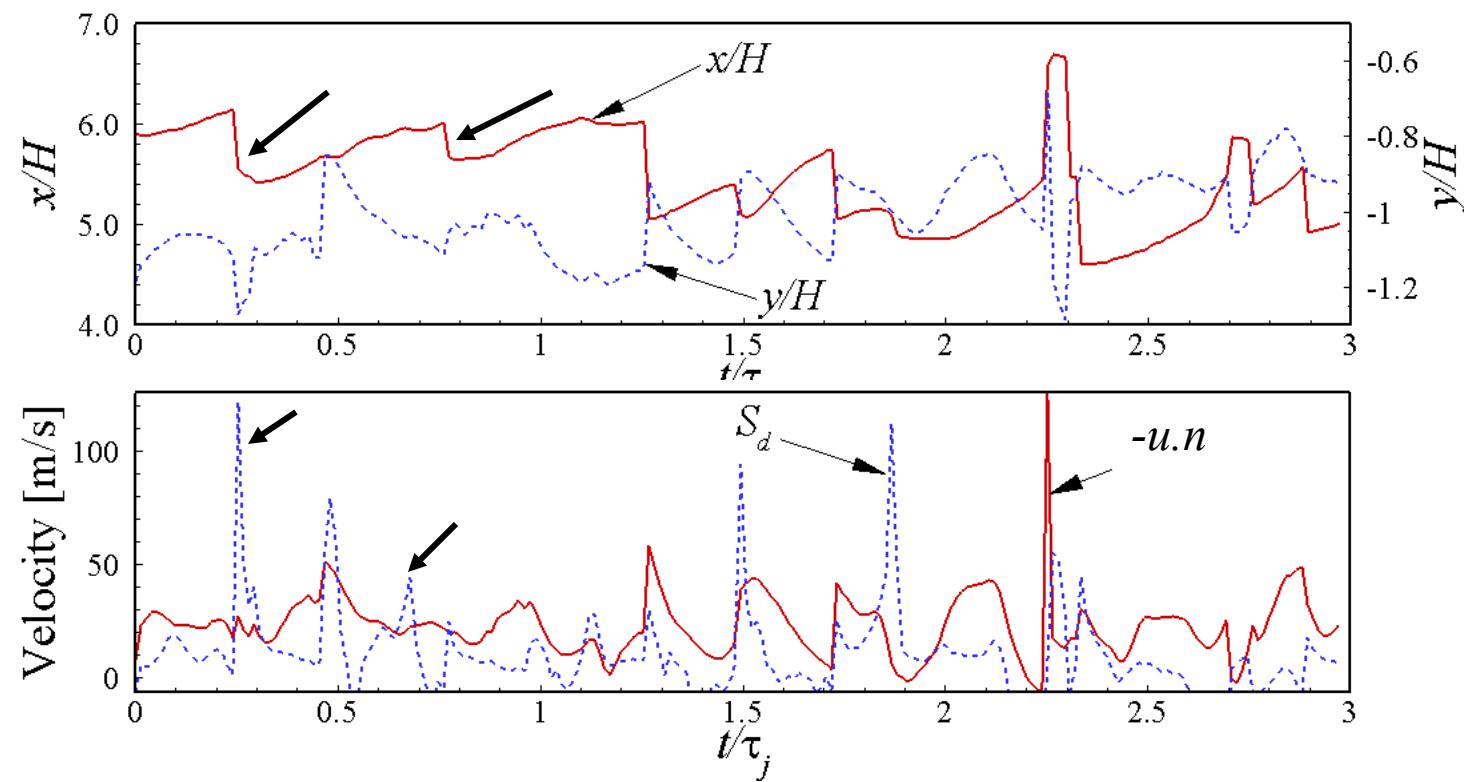


Temporal Evolution of OH at Stabilization Point



Temporal evolution of OH mass fraction isocontour at $t/\tau_j = 0.227 \sim 1.160$

Temporal Tracking of Stabilization Point



A priori Study of Combustion Models: Second-order Conditional Moment Closure for RANS

Analysis of 2nd Order CMC Applied to an Autoignitive H₂ jet flame*

CMC2 models
conditional means and
conditional variances
and covariances.

- Suggests framework for fundamental study of composition fluctuations.
- Illustrates how these fluctuations arise.

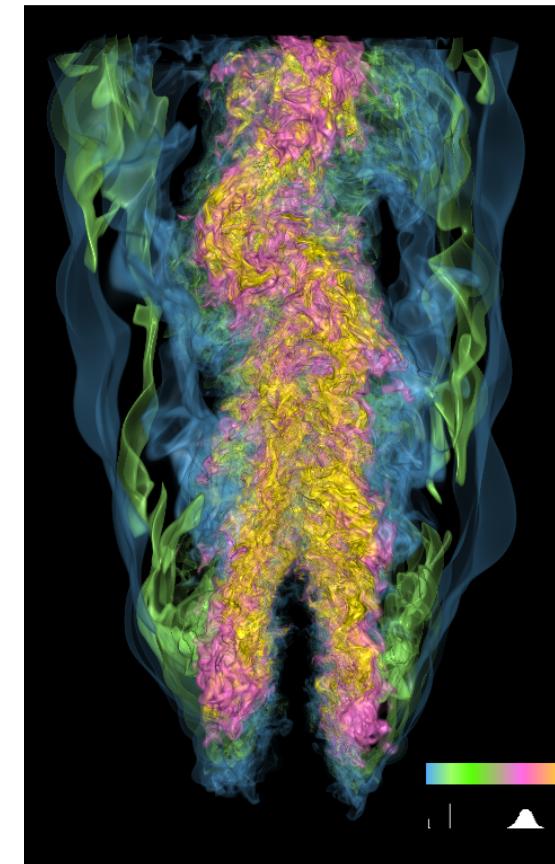
Examination of physics
indicates appropriate
simplifications

- Reduction of (co)variance matrix.
- Necessity of 2nd order closure.

Validation

- Testing of existing/
proposed sub-models/
modeling strategies

Volume rendering of HO₂ mass fraction in an autoigniting H₂ jet flame



* E.Richardson, C.S. Yoo, and J.H. Chen. Proc. Combust. Inst. 2009

Second-order CMC: Reaction Rate Closure

Solve for conditional average mass fractions:

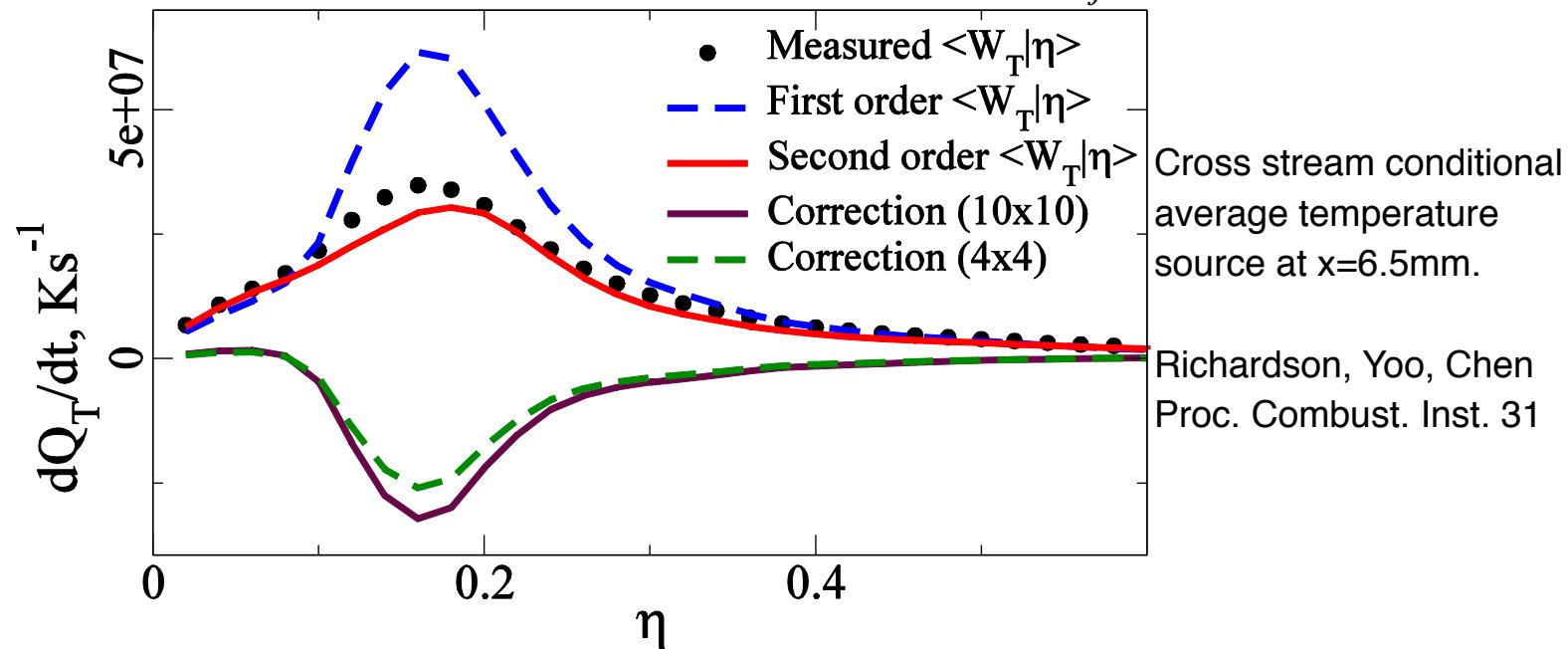
$$Q_i = \langle Y_i | \eta \rangle$$

1st order

2nd order

With reaction closure:

$$\langle W(Y) | \eta \rangle \approx W(Q) + \frac{1}{2} \frac{\partial^2 W}{\partial Y_i \partial Y_j} \Big|_Q \langle Y_i Y_j | \eta \rangle$$



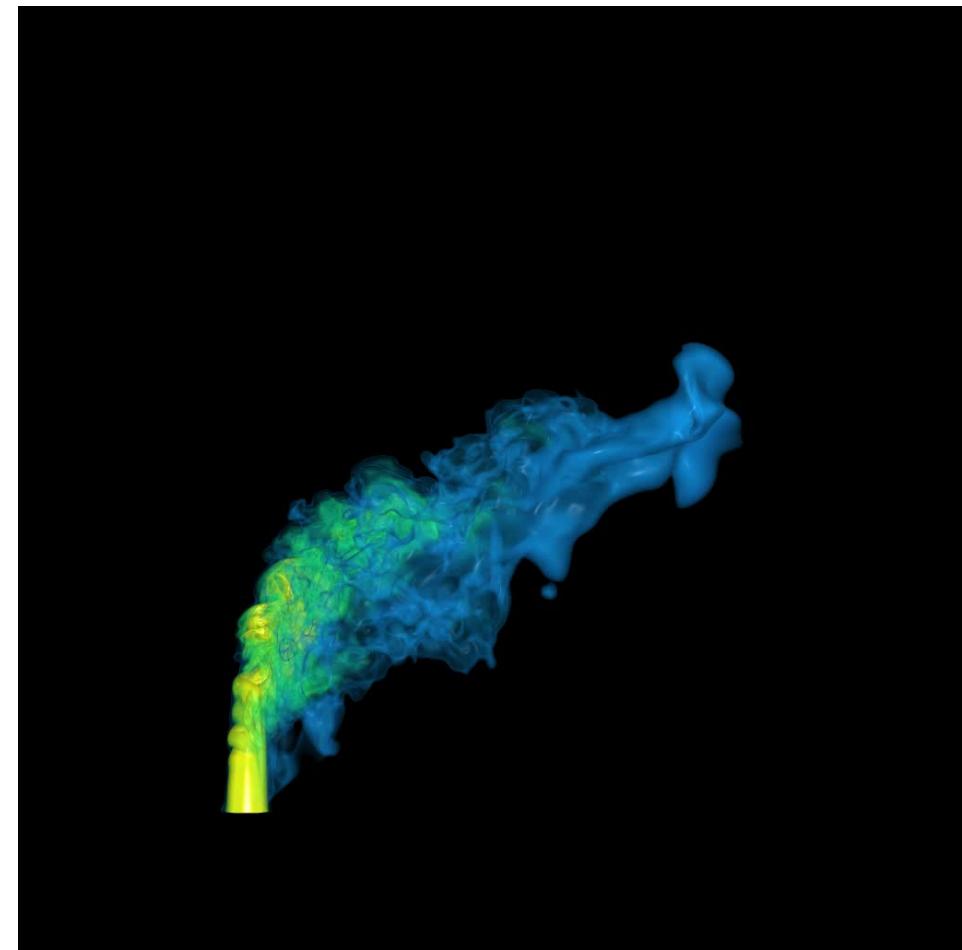
- 1) Need to include effects of conditional fluctuations in turbulent autoignition.
- 2) Second order contribution dominated by T, H, H_2, OH conditional co-variances.

Role of DNS – Case Studies

- Homogeneous Charge Compression Ignition (HCCI) Combustion
- Turbulent Jet Flames in Heated Co-Flow
- **Turbulent Jet Flames in Cross-Flow**

H₂/Air Reacting Jet in Crossflow

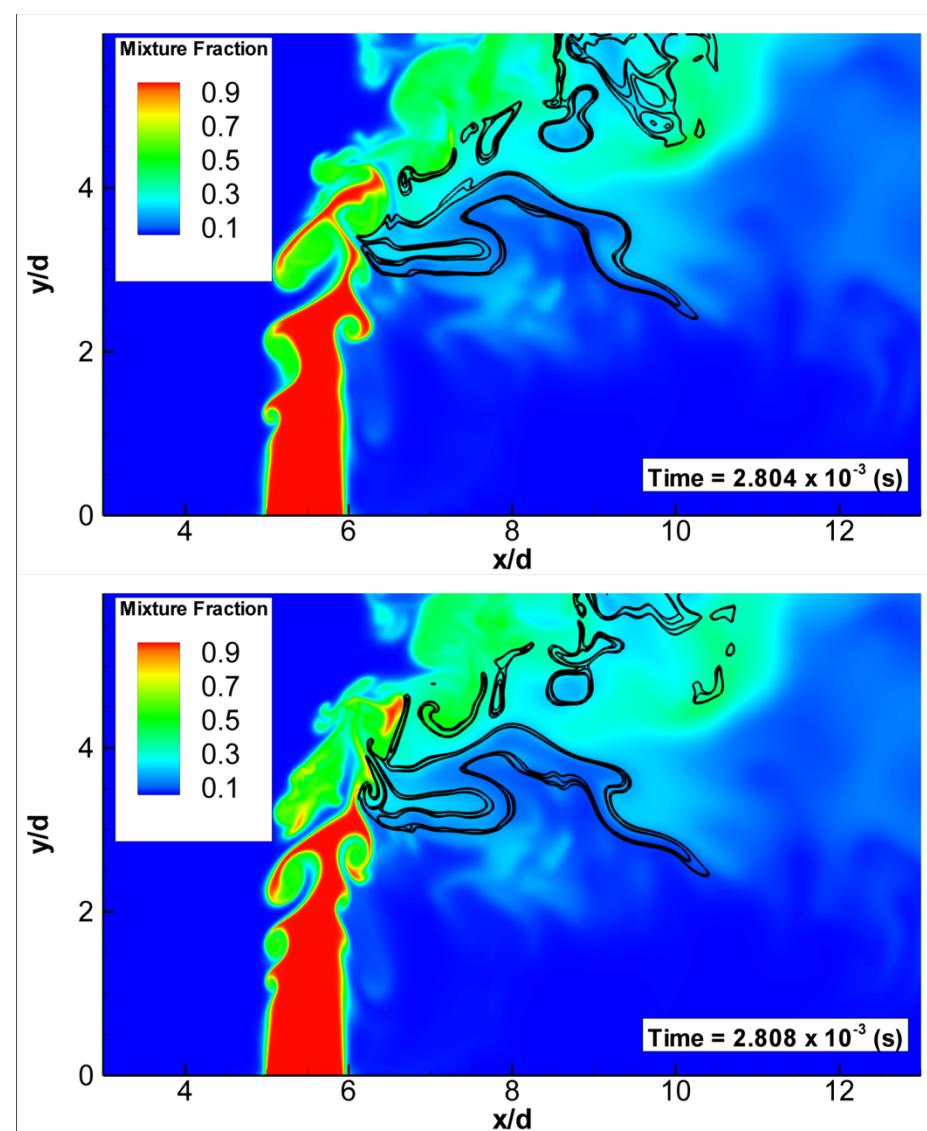
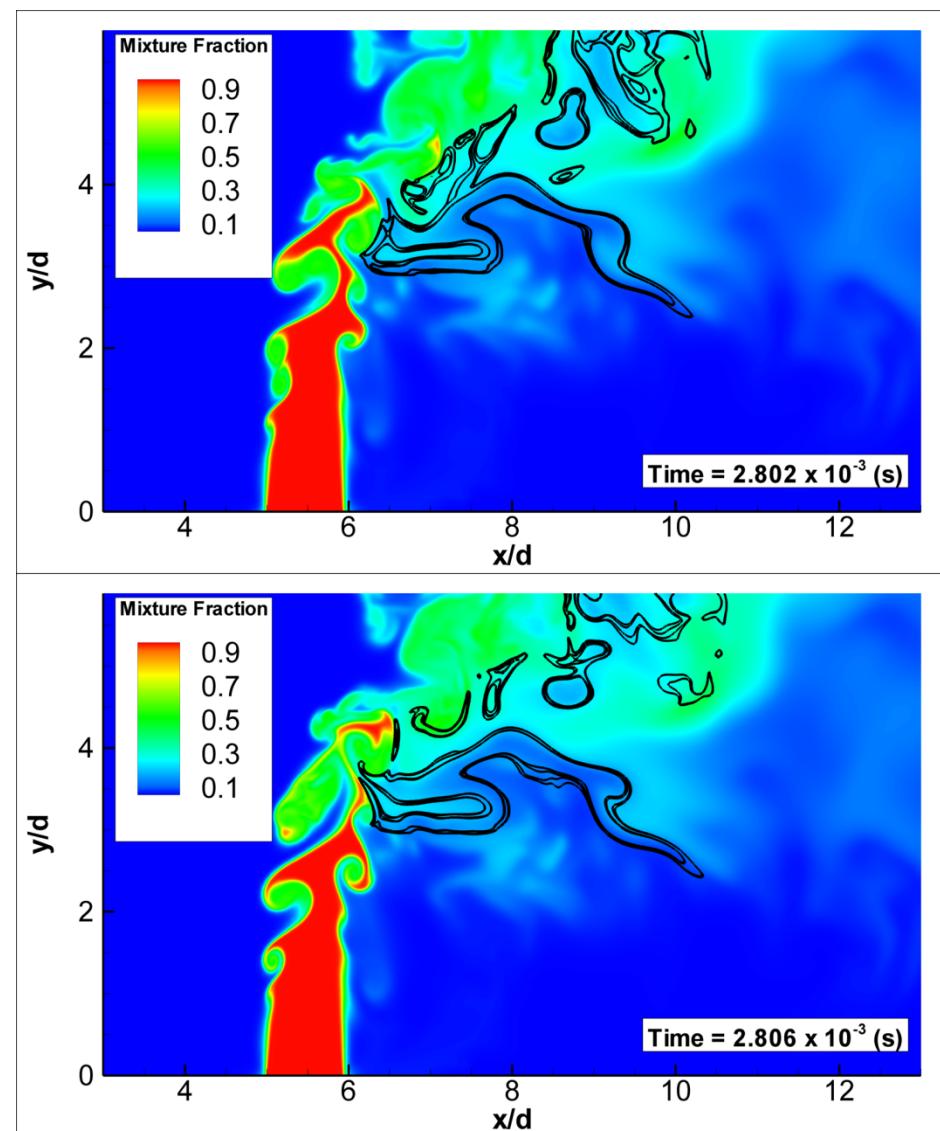
- JICF configuration relevant in many practical combustion applications.
- Complex 3D flow structures enhance mixing (shear layer vortices, counter-rotating vortex pair, horseshoe vortices, wake vortices)
- Mechanism of flame stabilization not well understood.

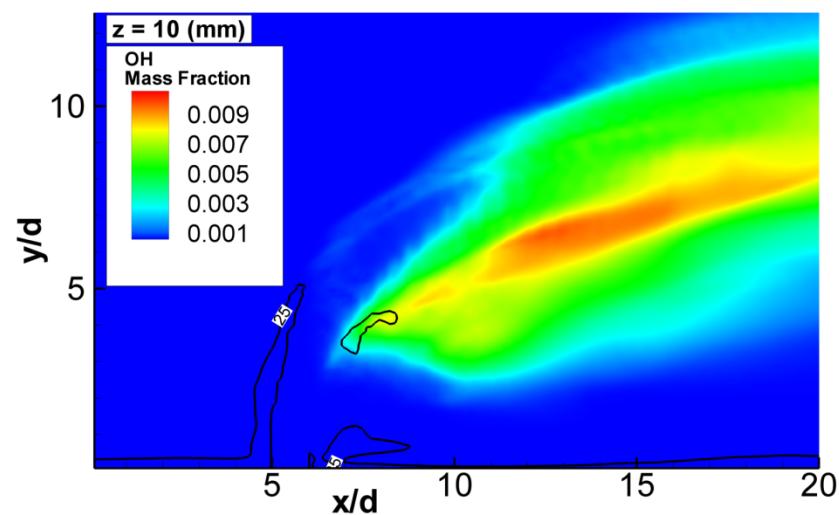
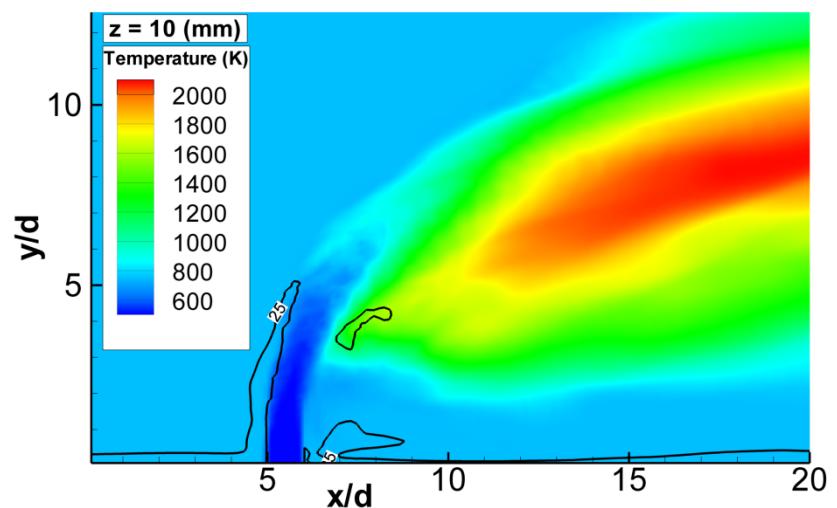
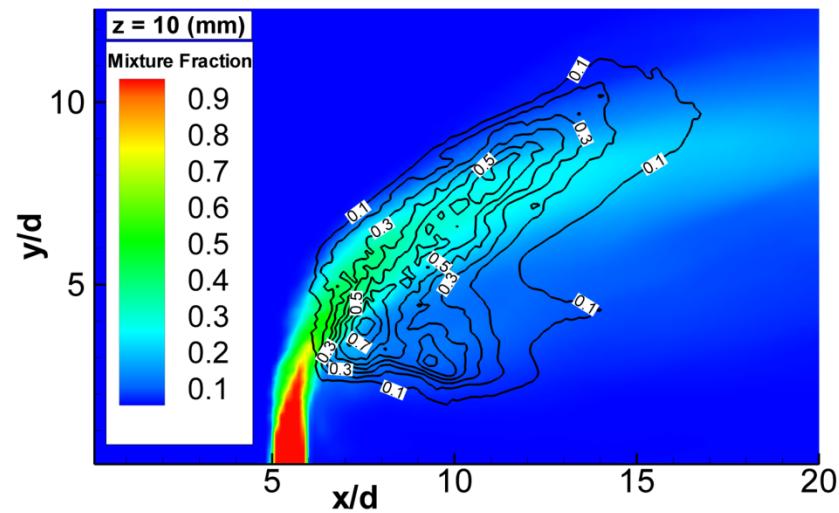
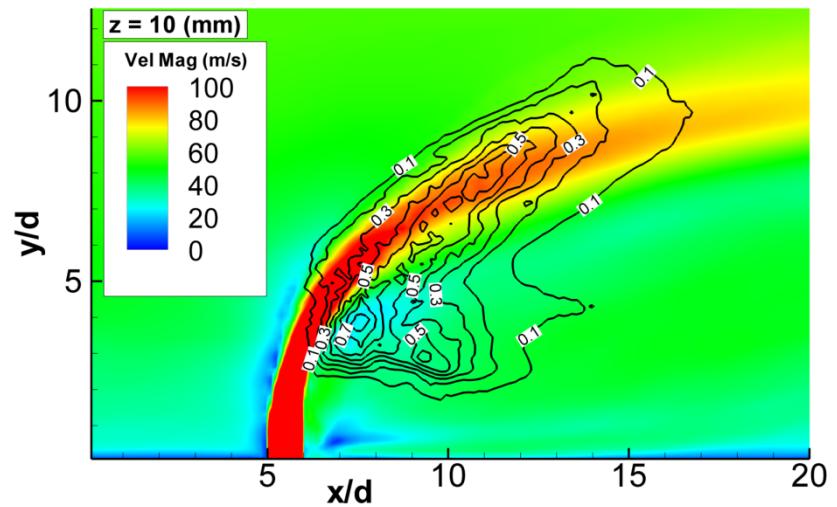


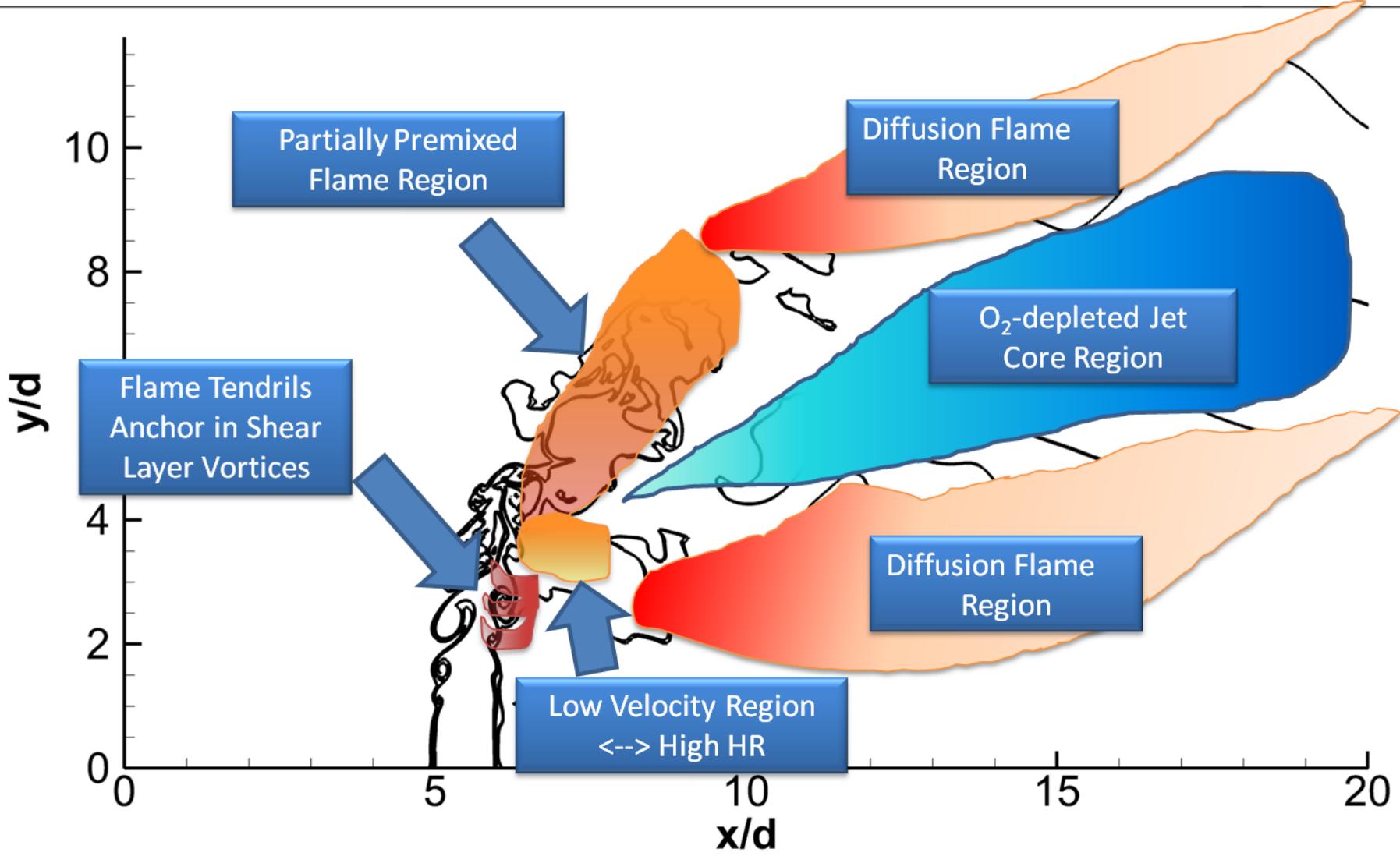
Volume rendering of H₂ in a reactive jet-in-crossflow by H. Yu of SNL

Introduction

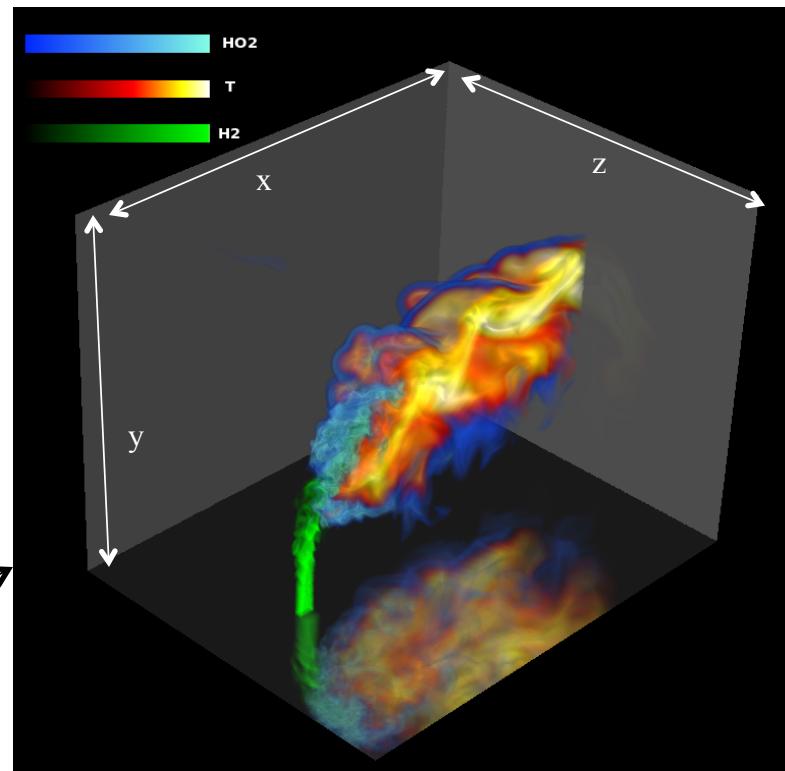
- Motivation: intrinsic flashback safety is critical for fuel injection system.
- Need to understand mechanisms of flame stabilization.
- Parametric studies investigating influence of nozzle shape, injection angle, momentum ratio, turbulence levels, and fuel flexibility (syngas).
- Present work focuses on injection angle variation only.
- Methodology: fully resolved 3D direct numerical simulation (DNS) with detailed chemistry.







Problem configuration



$\text{H}_2\text{-N}_2$ (7:3), 420 K
circular nozzle (1 mm dia)

	<u>90°</u>	<u>75°</u>
u_j (m/s)	250	258.8
Mom. ratio	12.5	13.4



Computational details

	X	Y	Z
Domain size (mm)	25	20	20
Grid points	1408	1080	1100
Resolution (μm)	17.8	18.2	10.2-24.3
Boundary conditions	inflow, outflow	no-slip wall, outflow	periodic

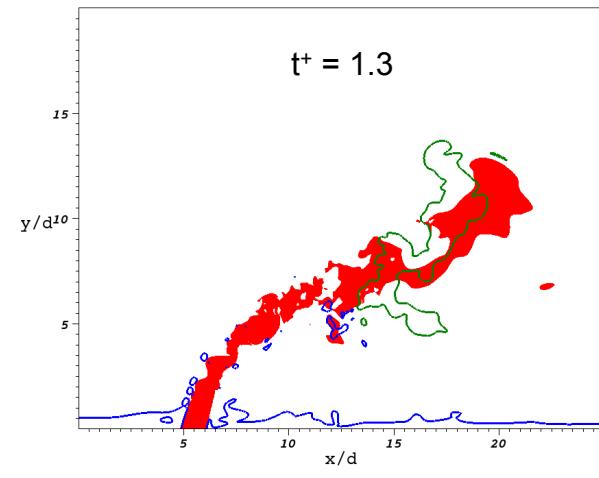
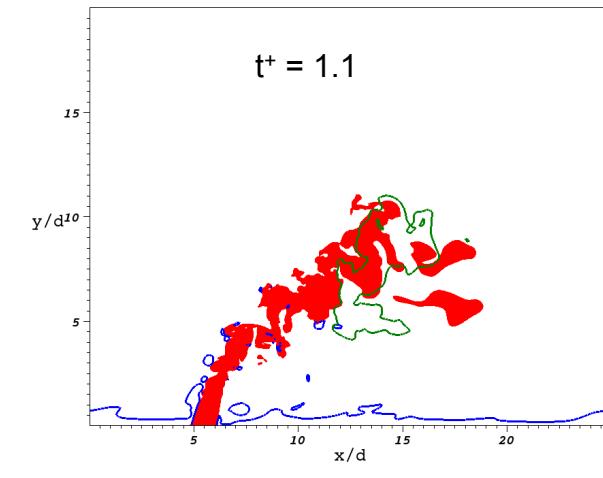
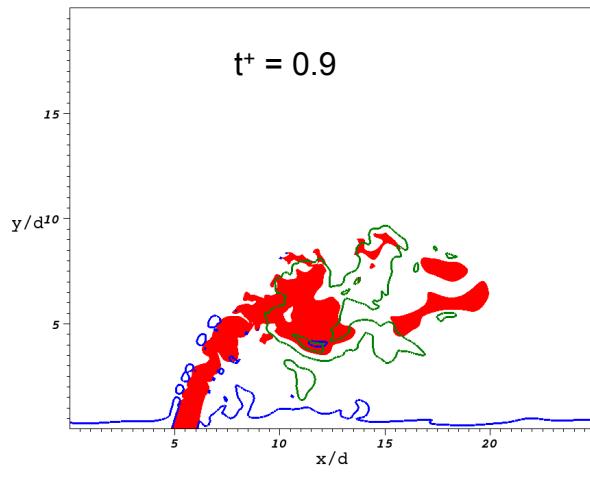
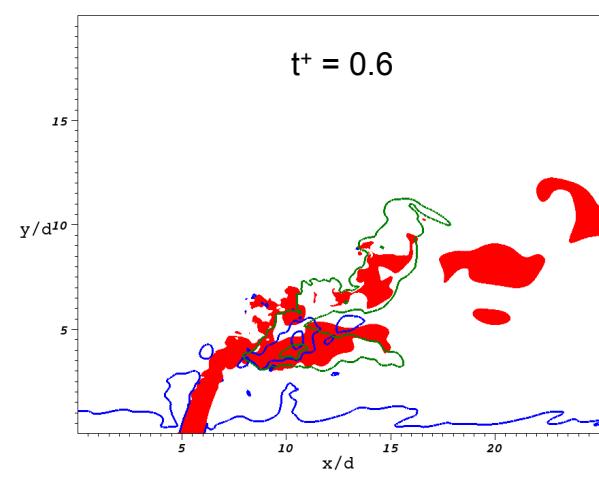
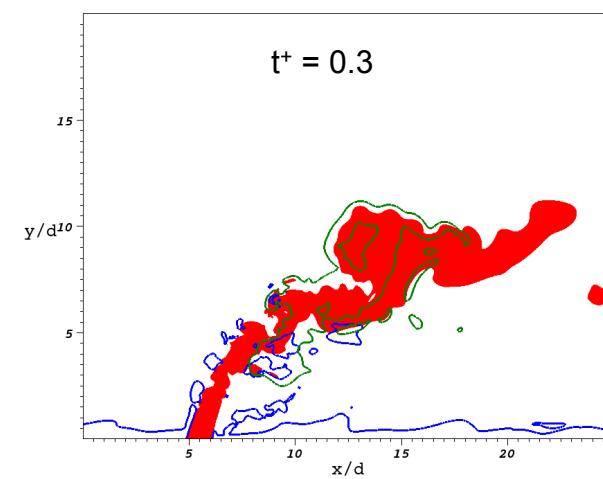
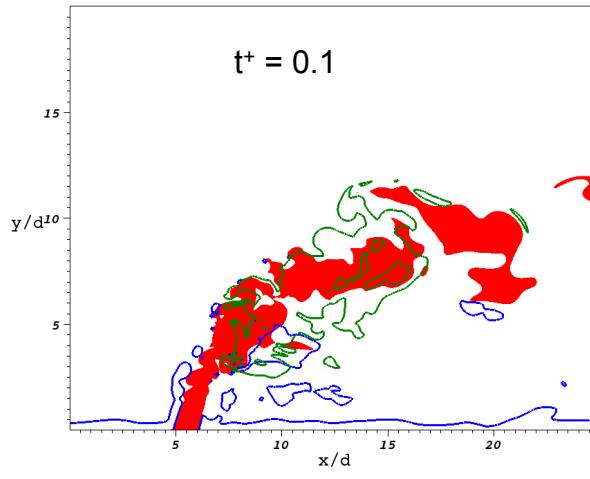
- DNS code S3D [1].
- Auxiliary inert DNS for inlet turbulence [2].
- Mechanism of Li *et al.*, [3] (9 species, 19 reactions).
- Solution advanced with constant $\Delta t = 4$ ns

[1] Chen *et al.* 2009, *Comp. Sci. Disc.* **2**-015001.

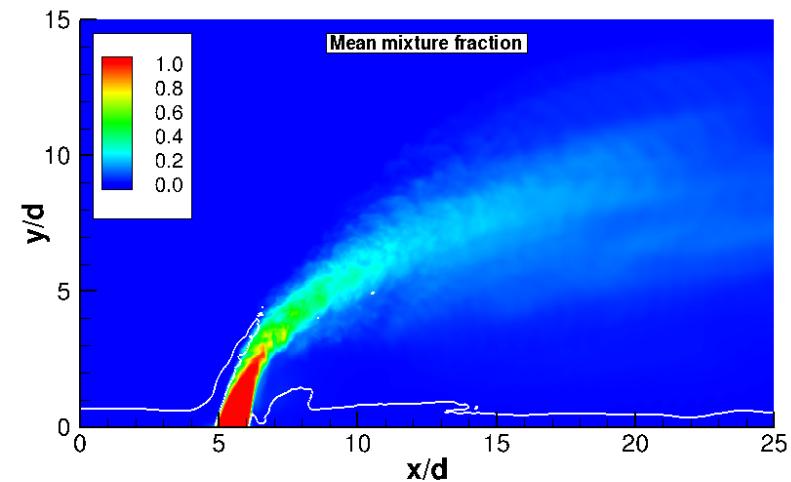
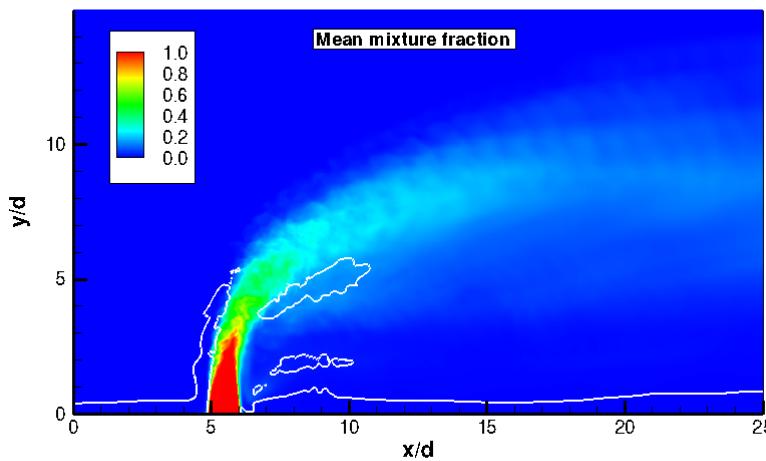
[2] Grout *et al.* 2011, *Proc. Comb. Inst.*, **33**.

[3] Li *et al.* 2004, *Int. J. Chem. Kin.*, **80**.

Temporal Evolution of Heat Release, Velocity, Mixture Fraction – 75° case



Analysis – 75° case

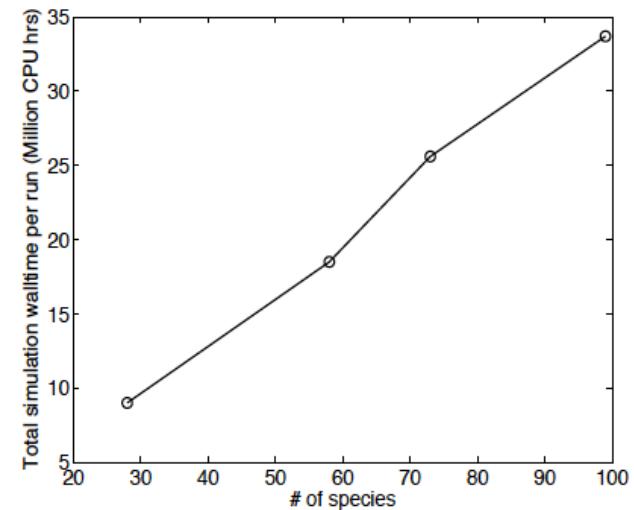


- Low velocity region close to flammable mixture appears critical for flame stabilization.
- Evident from average field quantities.
- Inert flow data might not be sufficiently indicative as velocity field is influenced by heat release (Hasselbrink & Mungal 2001, *J. Flu. Mech. 443*).

Combustion Science on a 10-20 Pflop Hybrid Many-Core Machine (Titan) – 1. More Chemistry

Increased Chemical Kinetic Complexity for low temperature, high pressure:

- 9-22 species Jaguar (H₂, syngas, methane, ethylene)
- 60-100 species Titan (nheptane, iso-octane, biofuels)



Fuel	Species	Unit Cost (us)	Total cost (million CPU hrs)
Ethanol	28	370	9.0
N-Heptane	58	760	18.5
Biodiesel	73	1050	25.6
Iso-octane	99	1380	33.7

Combustion Science on a 10-20 Pflop Hybrid machine (Titan) – 2. Higher Reynolds number

Maintaining simple chemistry, increase dynamic range of fluid scales by increasing mesh size (Reynolds number)

- 9-22 species Jaguar (H_2 , syngas, methane, ethylene) increase the turbulent Reynolds number in a laboratory scale jet flame – better validation data for model assessment