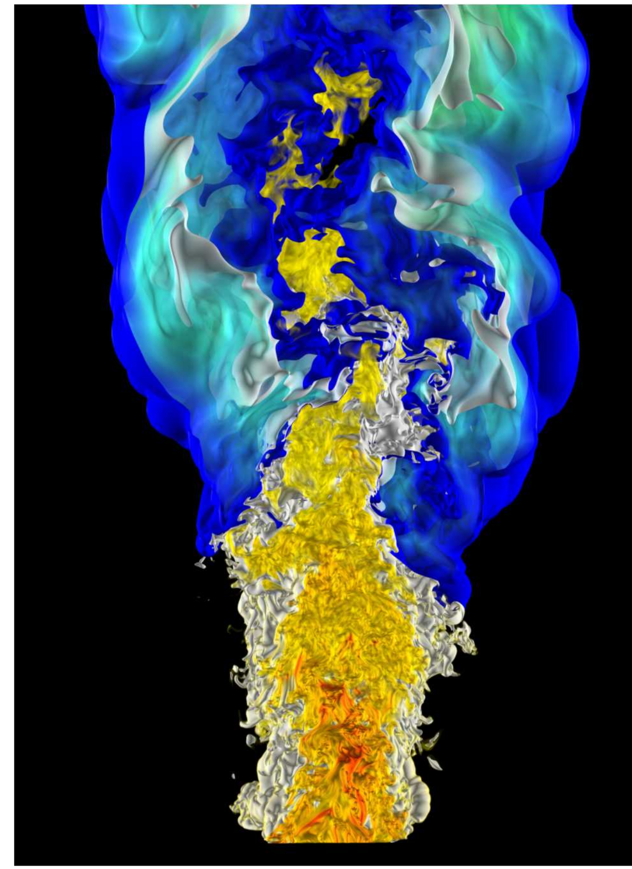
DNS of Turbulent Combustion in Complex Flows

SAND2019-6404C

Jacqueline H. Chen

Sandia National Laboratories

jhchen@sandia.gov



11th Mediterranean Combustion Symposium

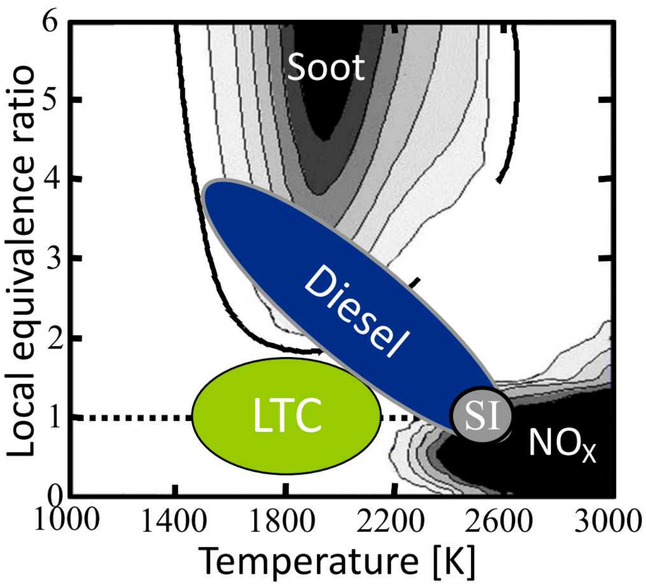
Tenerife, Spain

June 16-20, 2019

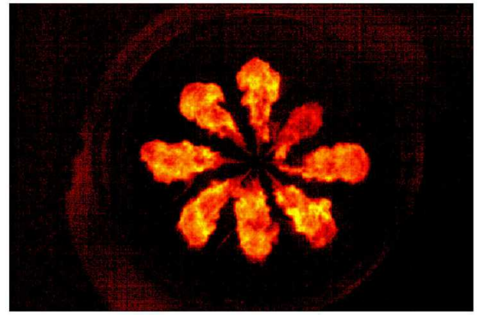
Office of Science
U.S. Department of Energy

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

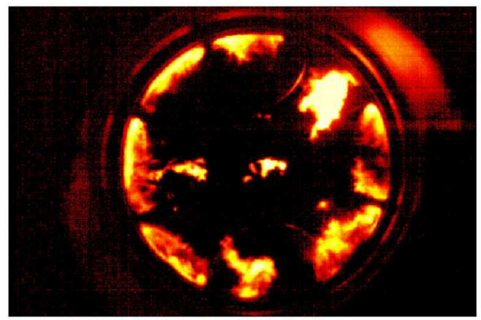
Autoignition and Flame Stabilization in Engines

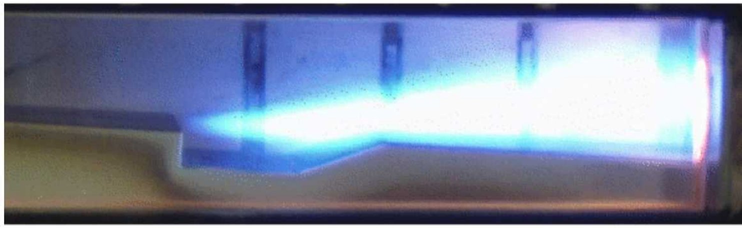


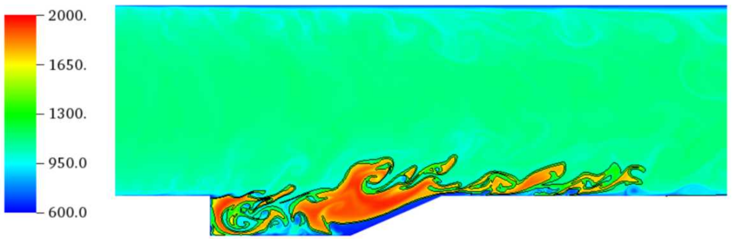
Conventional diesel *

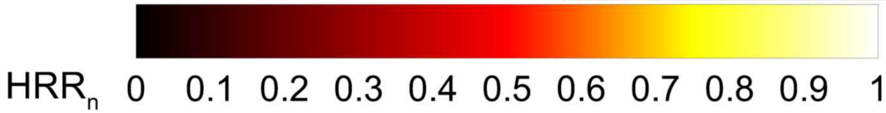


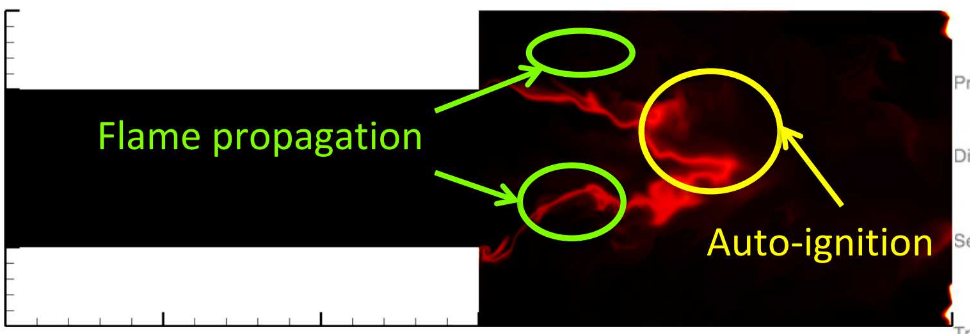
Early injection PCCI

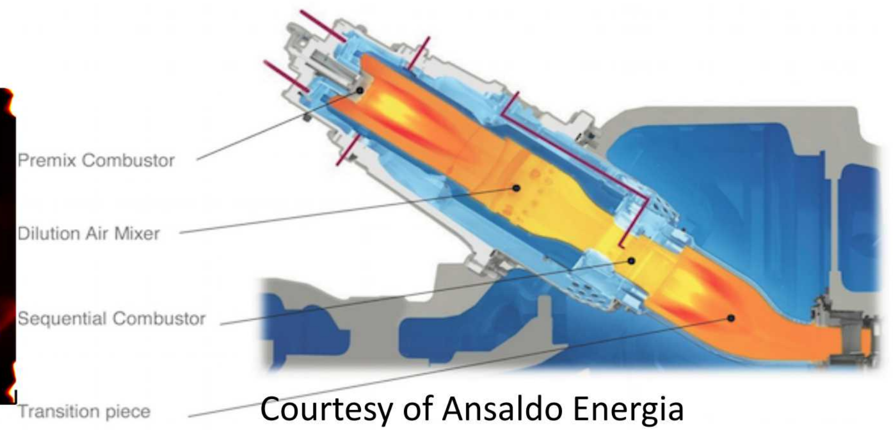








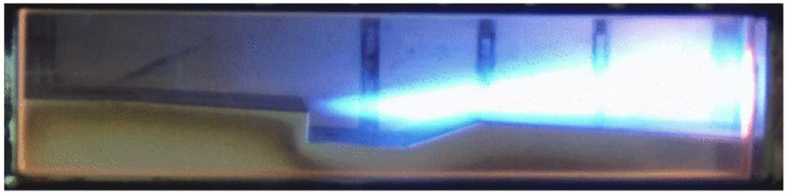


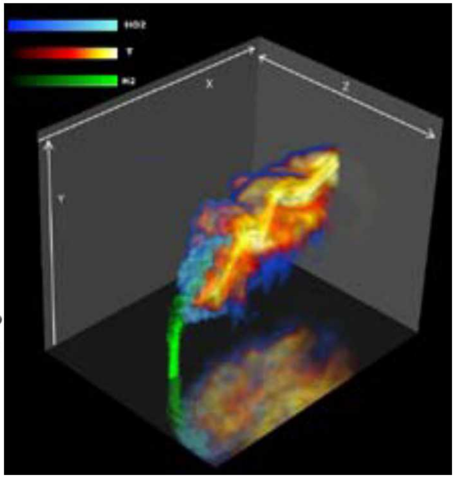


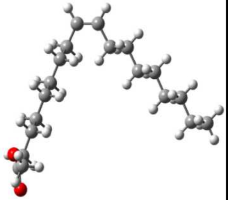
Courtesy of Ansaldo Energia

Exascale Simulation of Turbulent Combustion

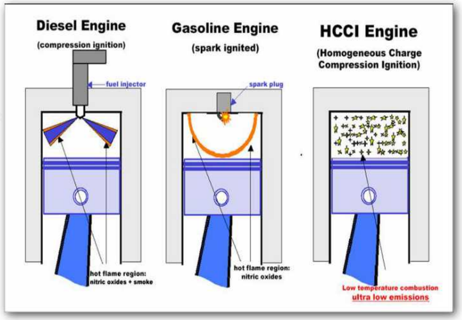
- Fundamental insights into multi-physics in highly turbulent flames to formulate physics-based LES models





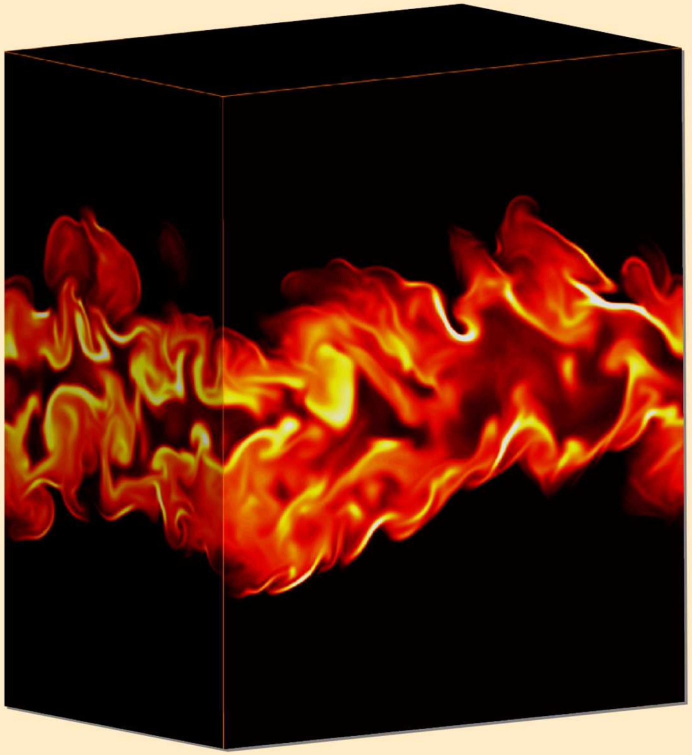


- High Reynolds number, high pressure, large turbulent velocity fluctuations, compressibility
  - LES SGS closures inherited from nonreacting flows
  - Multi-scale energy transfer processes
  - Complex thermo-chemical trajectories through flames and ignition fronts
- High-fidelity direct numerical simulation (DNS) and hybrid DNS/LES methodologies
  - sufficient chemical fidelity to differentiate effects of fuels where there is strong turbulence-chemistry interactions
  - complex flows



Direct Numerical Simulation – S3D

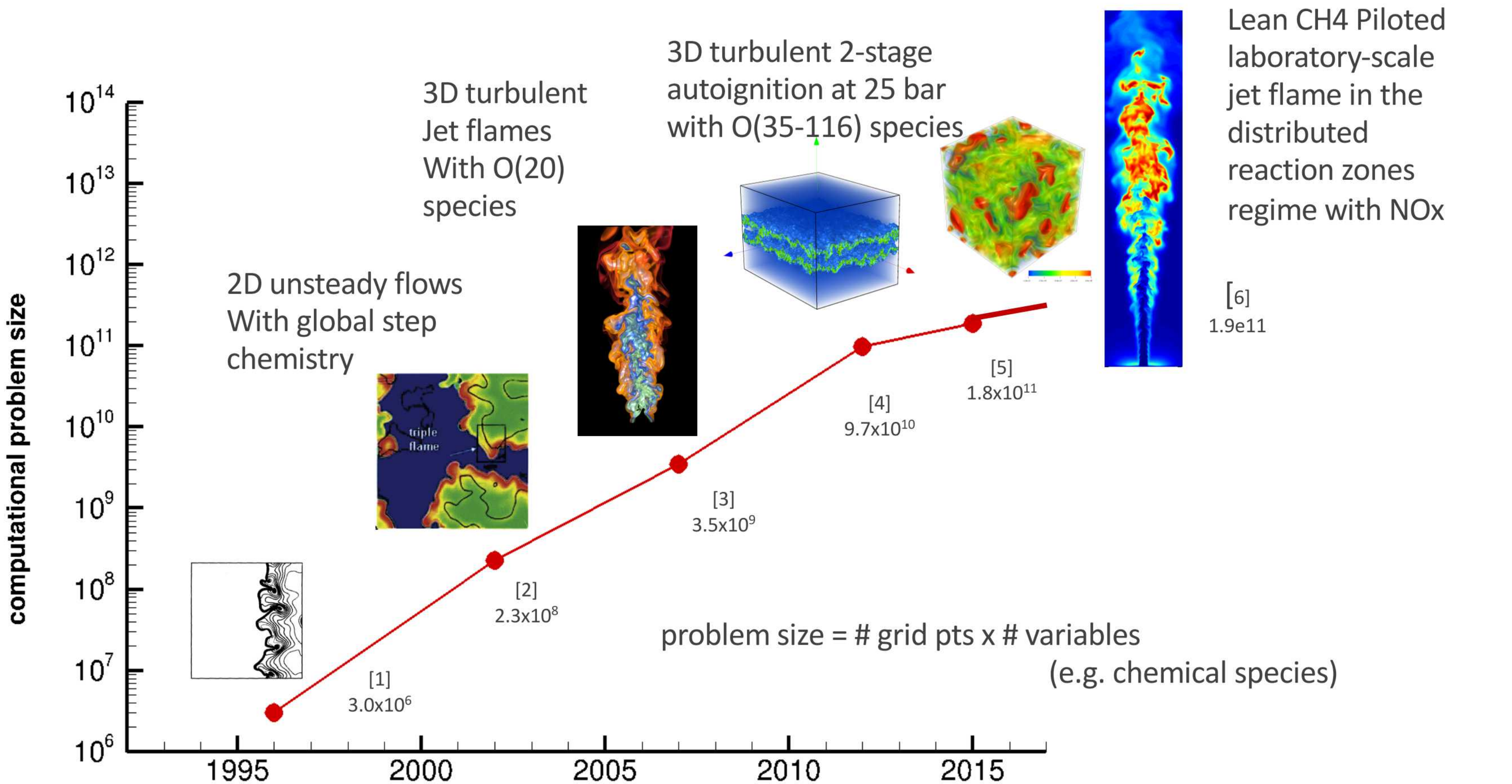
- **DNS of turbulent reacting flows**
- **Solves compressible reacting Navier-Stokes, total energy and species continuity equations**
- **High-order finite-difference methods**
- **Detailed reaction kinetics and molecular transport models**
- **Lagrangian particle tracking (tracers, spray, soot)**
- **In situ analytics and visualization**
- **Refactored for multi-threaded, many core heterogeneous architectures**



DNS provides unique fundamental insight into the chemistry-turbulence interaction

Chen *et al.*, *Comp. Sci. Disc.*, 2009

Computational intensity of DNS scales with Moore's Law



[1] T. Echekki, J.H. Chen, *Comb. Flame*, 1996, vol.106.

[2] T. Echekki, J.H, Chen, *Proc. Comb. Inst.*, 2002, vol. 29.

[3] R. Sankaran, E.R. Hawkes, J.H. Chen, *Proc. Comb. Inst.*, 2007, vol. 31.

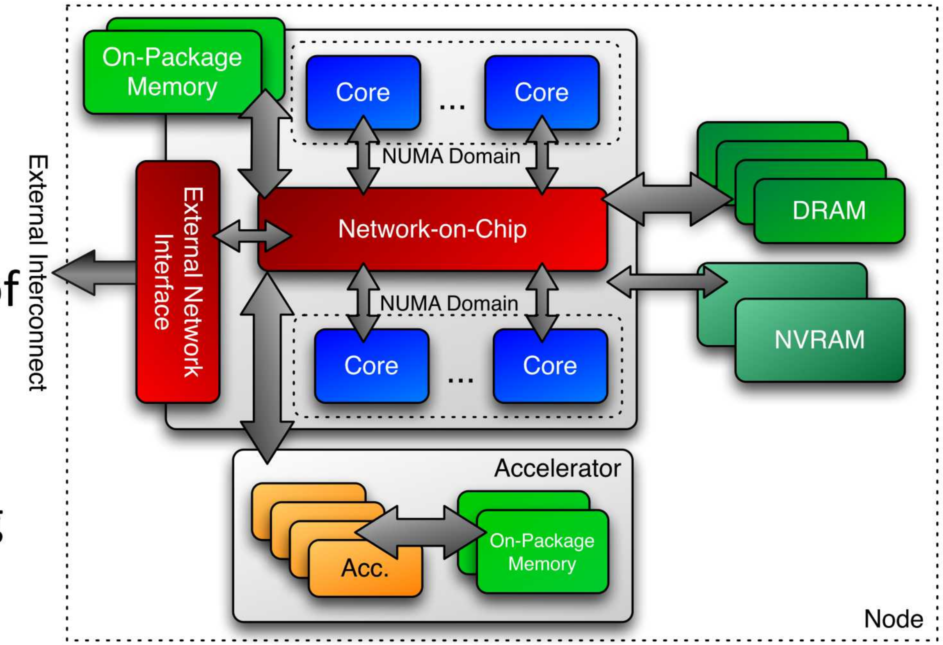
[4] E.R. Hawkes, O. Chatakonda, H. Kolla, A.R. Kerstein, J.H. Chen, *Comb. Flame*, 2012, vol. 159.

[5] 2015 submission for Gordon Bell prize

[6] H. Wang, E. Hawkes, J. H. Chen, Comb. Flame 2017

Constraints imposed by exascale architecture

- **Power:** primary design constraint for future HPC system design
- **Cost:** Data movement dominates: optimize to minimize data movement
- **Concurrency:** Exponential growth of parallelism within chips
- **Locality***:* must reason about data locality and possibly topology
- **Memory Scaling**: Compute growing 2x faster than capacity or bandwidth,
- **Heterogeneity:**Architectural and performance nonuniformity

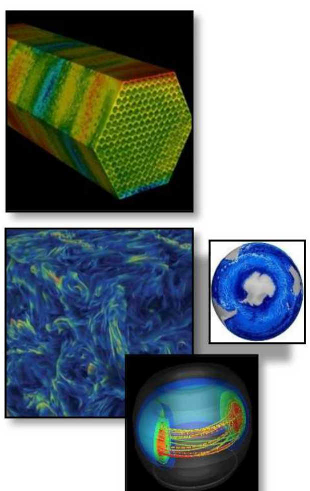


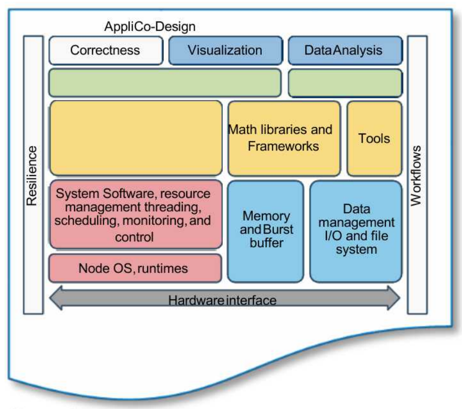
Conceptual model of future HPC node

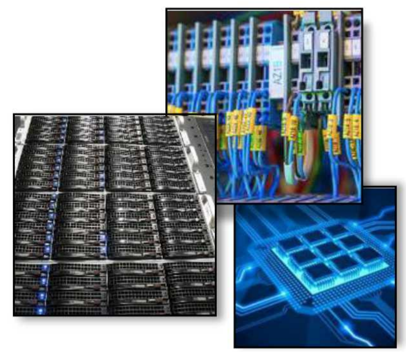
Express data locality and independence, express massive parallelism, minimize data movement and reduce synchronization, detect and address faults

DOE Exascale Computing Project (ECP) will achieve capable exascale machines in 2021-2023

Application Development	Software Technology	Hardware Technology	Exascale Systems
Science and mission applications	Scalable and productive software stack	Hardware technology elements	Integrated exascale supercomputers





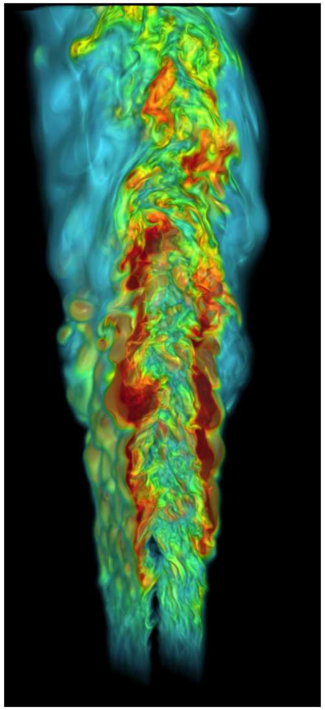


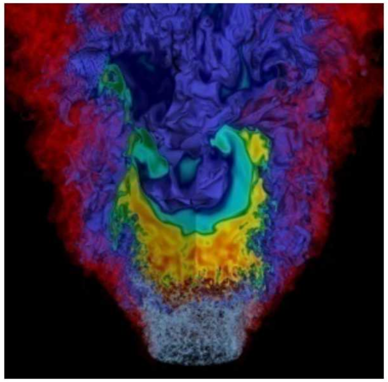
ECP's work encompasses applications, system software, hardware technologies and architectures, and workforce development

From Paul Messina's ASCAC talk April 19, 2017

ECP application: transforming combustion science and technology through exascale simulation (Pele)

PeleC and PeleLM: Block-structured adaptive mesh refinement, multi-physics: spray, soot, and radiation, real gas, complex geometry





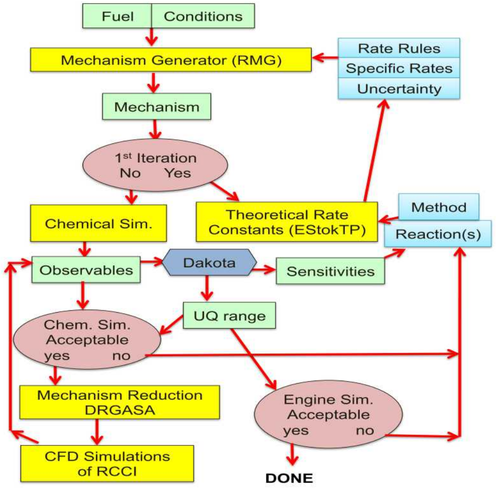
Effects of reactivity stratification at:

- high pressure
- high turbulence
- fuel blends

on:

- ignition delay
- combustion rates
- emissions

Automated Mechanism Generation



S3D: multi-block compressible reacting DNS multi-physics validation: spray, soot, radiation

Argonne NATIONAL LABORATORY · BERKELEY LAB Lawrence Berkeley National Laboratory · OAK RIDGE National Laboratory · Sandia National Laboratories · NREL NATIONAL RENEWABLE ENERGY LABORATORY

Outline

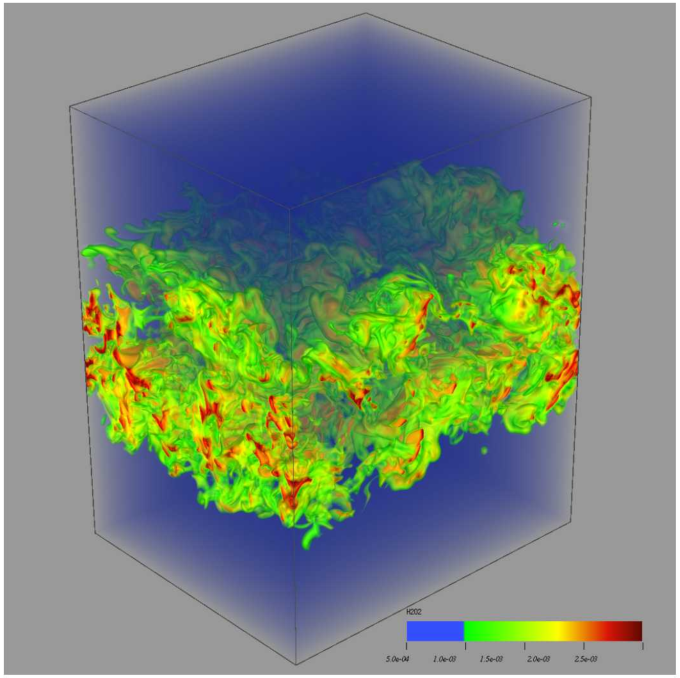
- Examples of DNS of turbulent combustion relevant to engines:
  - DNS of turbulent autoigniting nDodecane diesel jets (S3D and PeleLM)
  - DNS of high-speed flame stabilization behind a step
  - DNS of reheat combustion in staged gas turbines
- Path to Exascale Combustion Simulations (2021-2023)
  - Programming models
  - Composable in situ workflows (analytics, machine learning)
  - Unsupervised anomaly detection

DNS of a Turbulent Autoigniting n-Dodecane temporal jet at 25 Bar

Giulio Borghesi[1], Alex Krisman[1], Tianfeng Lu[2] and Jackie Chen[1]

[1]Combustion Research Facility, Sandia National Laboratories

[2]University of Connecticut

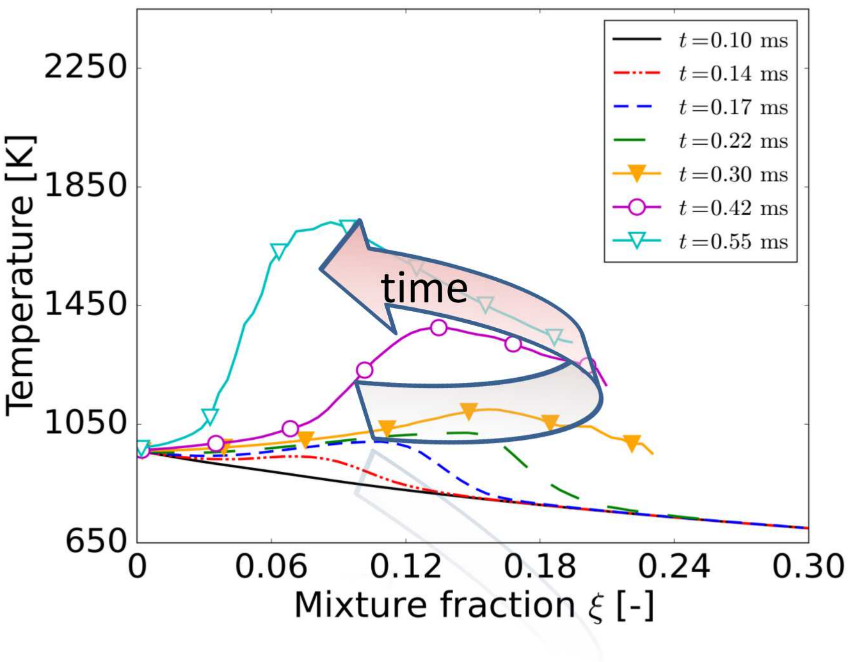


Ketohydroperoxide mass fraction

Borghesi et al. Combustion and Flame, 2018

Background and Objective

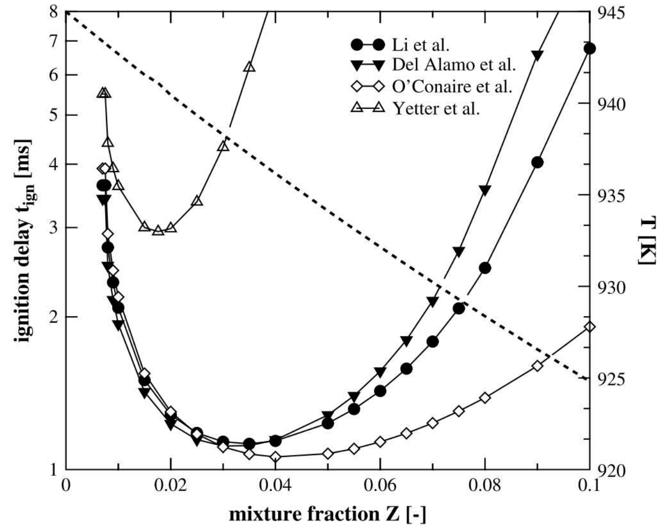
- Low-temperature combustion (LTC) aims at increasing fuel efficiency and reducing emissions
- Under LTC conditions, combustion occurs in a mixed mode and in multiple ignition stages
- Ignition is now very sensitive to the fuel chemistry, especially to the low temperature reactions branch



Question: How does transport and low-temperature chemistry affect ignition in low-temperature diesel combustion?

Background on high-temperature ignition

- Homogeneous PSR calculations show the existence of x value, x_m, where ignition delay has a minimum;
- Flamelet simulations show the ignition delay increases with scalar dissipation N until a critical value is reached;
- In practical systems, ignition occurs at locations close to x_m where N is low. The ignition delay is longer than in PSR;
- **Question:** which features of high-T ignition carry over to low-T ignition?



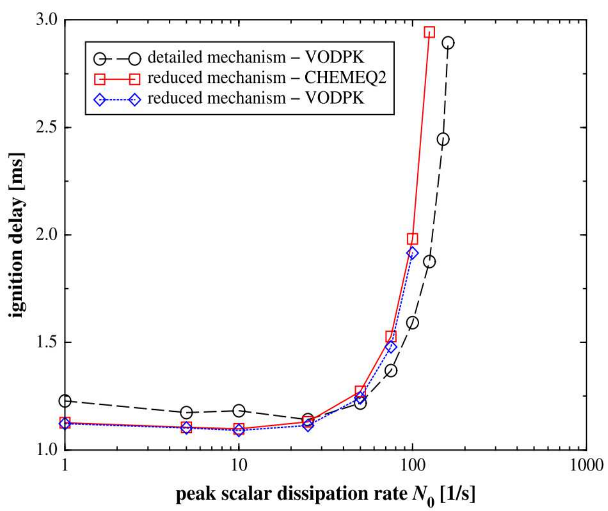
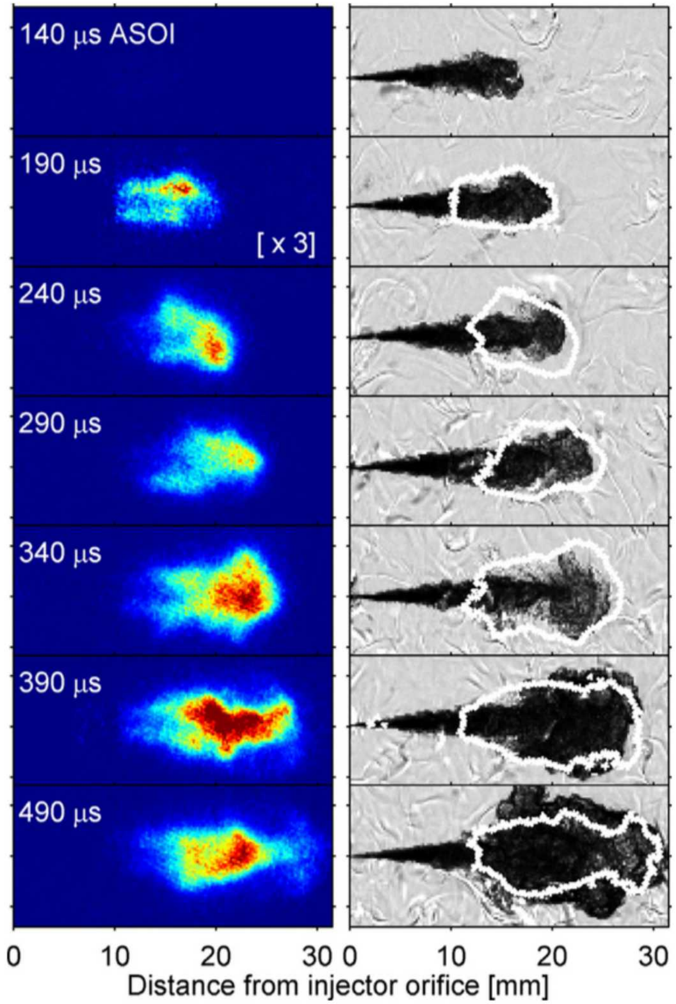


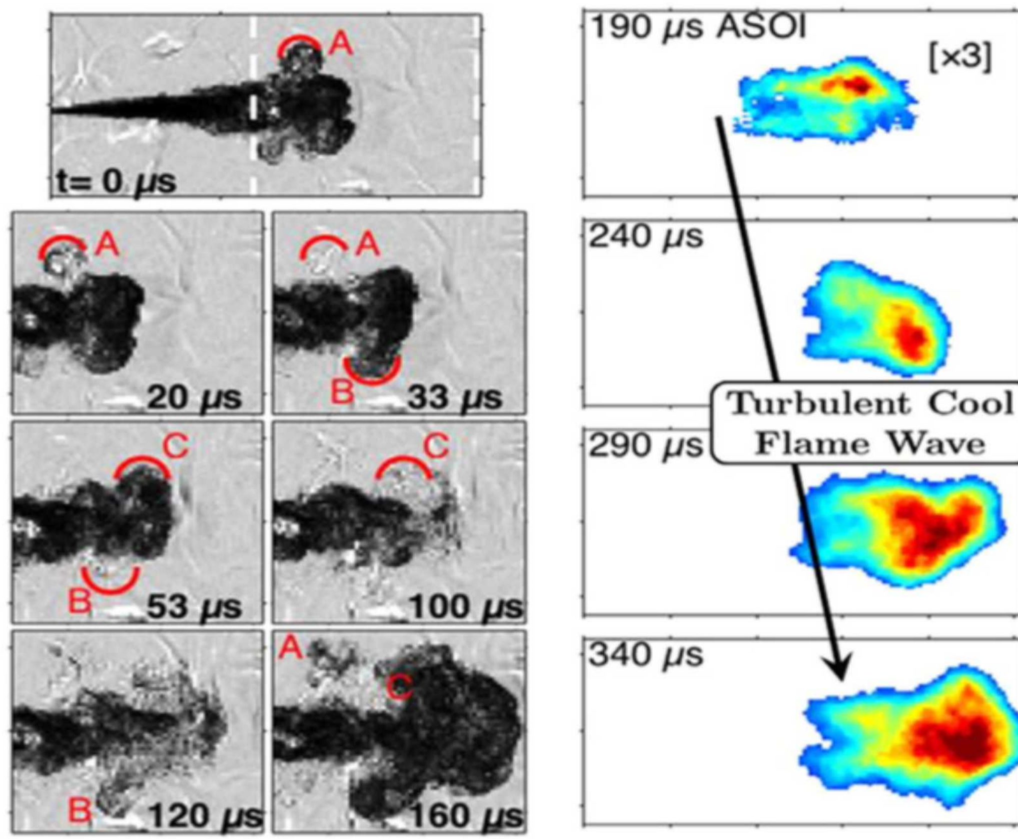
Figure: ignition delay time in PSR and in nonpremixed flamelet simulation[1]

[1] E. Mastorakos, PECS (2009), pp. 57-97

Low Temperature Diesel Combustion Experiments – Engine Combustion Network



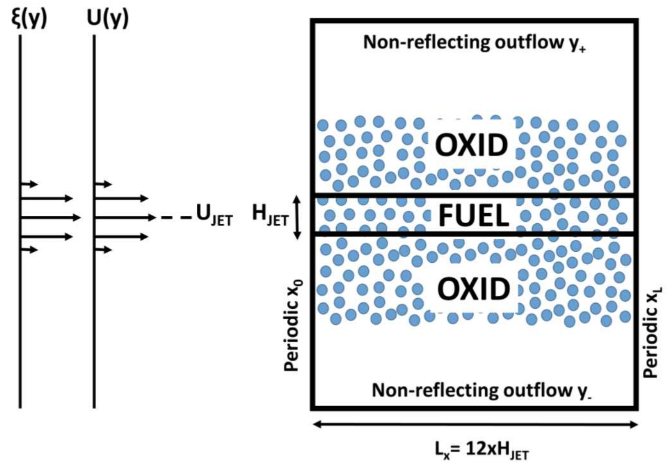
Skeen et al., PROCI 35 (2015) 3167-3174



Dahms et al., PROCI 36 (2017) 2615-2623

DNS Configuration and Physical Parameters

- **Pressure:** 25 bar
- **Air stream:** 15% X_{O2}+85% X_{N2}, T=960 K
- **Fuel stream:** *n*-dodecane at ξ=0.3, T=450 K
- **Kinetics:** 35-species non-stiff reduced (Lu)
- **Fuel jet velocity:** 21 m/s, Re_j = 7000, Re_t ~ 950
- **Code and cost:** S3D Legion, 60M CPUh
- **Setup:**
  - 3 billion grids
  - 3 microns spatial grid resolution
  - Dimensions: 3.6 mm x 14.0 mm x 3.0 mm
  - 1 ms of physical time with 4 ns timesteps to observe ignition and propagation of burning flames throughout the domain
  - BCs: X and Z periodic, Y NSCBC outflows



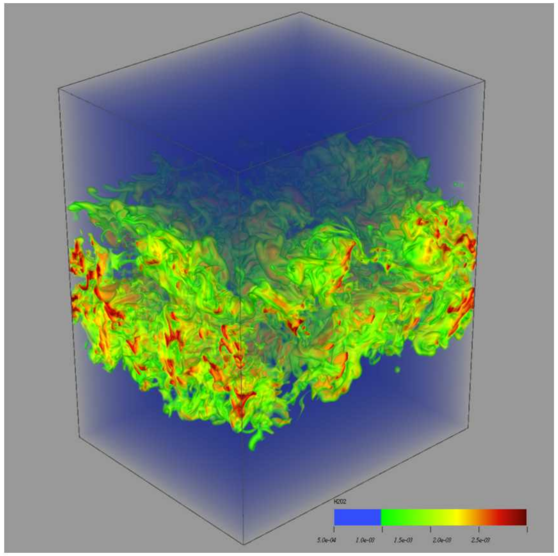
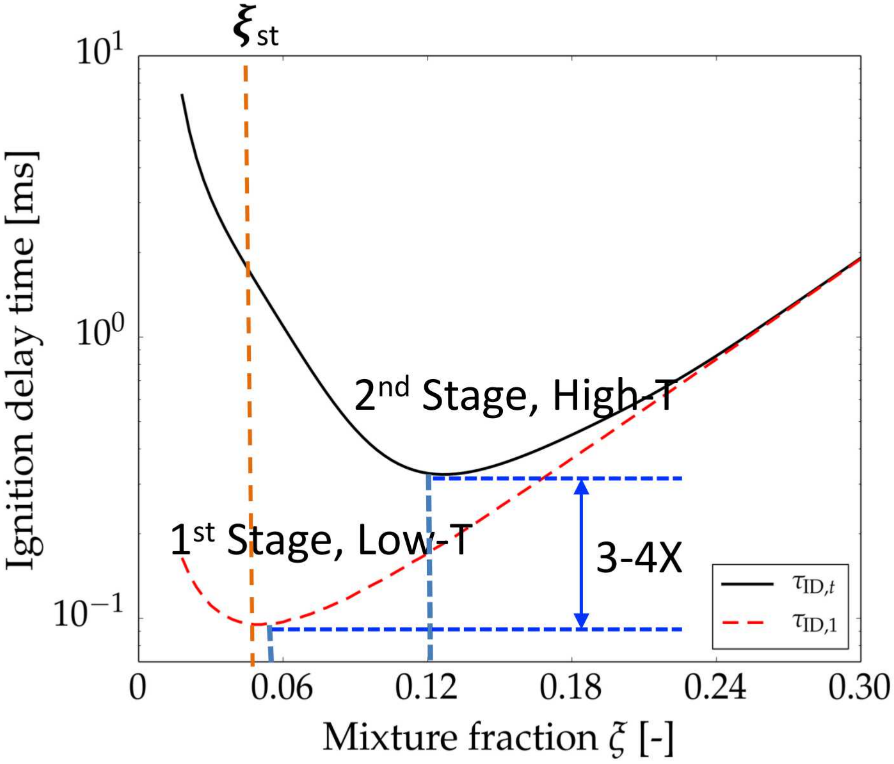
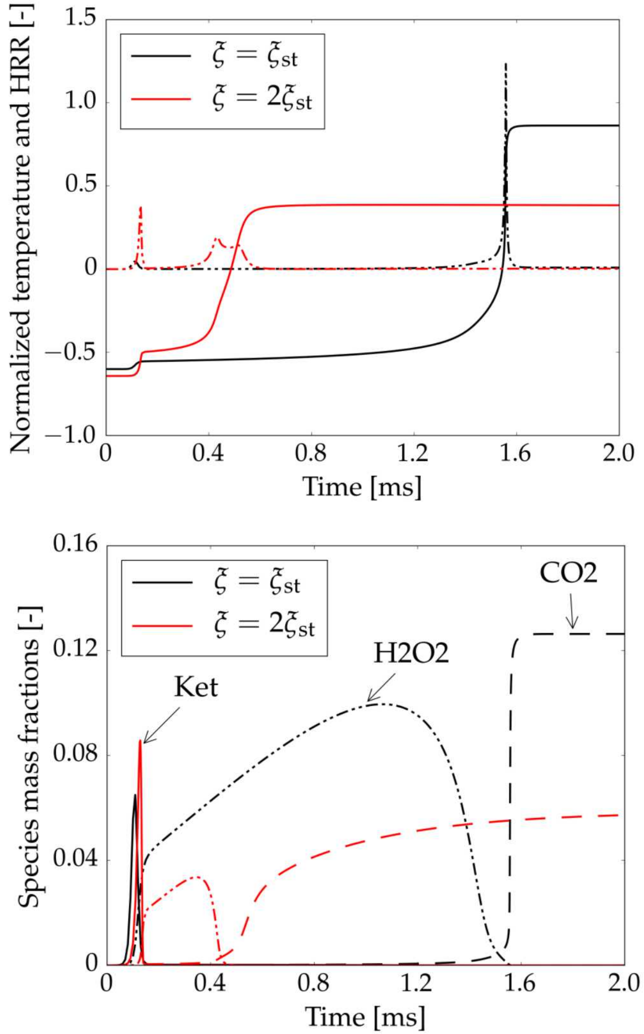


Figure: H_2O_2 mass fraction at t=0.17 ms after start of reactions

Homogeneous Multi-Stage Autoignition

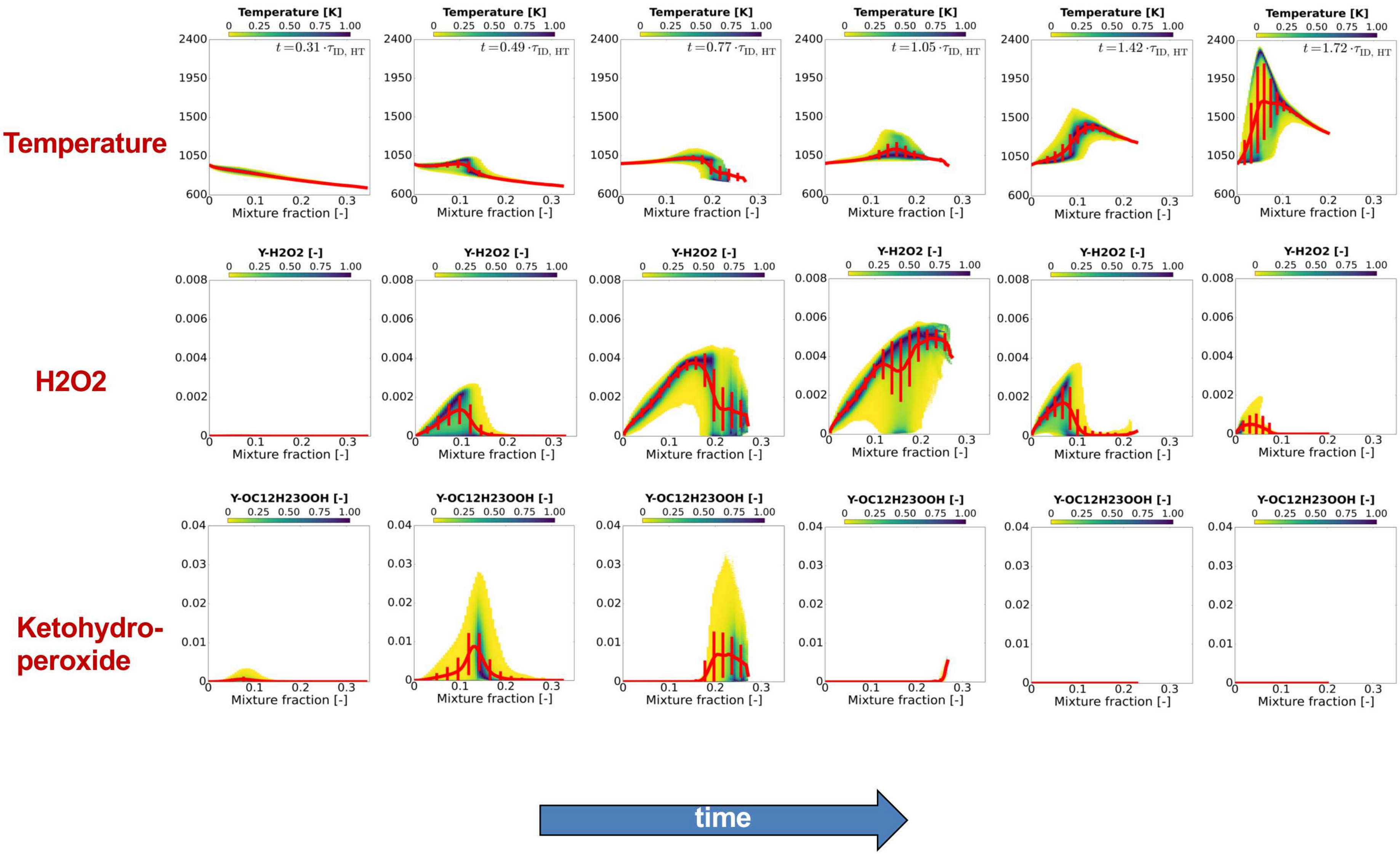


Homogeneous ignition delay time

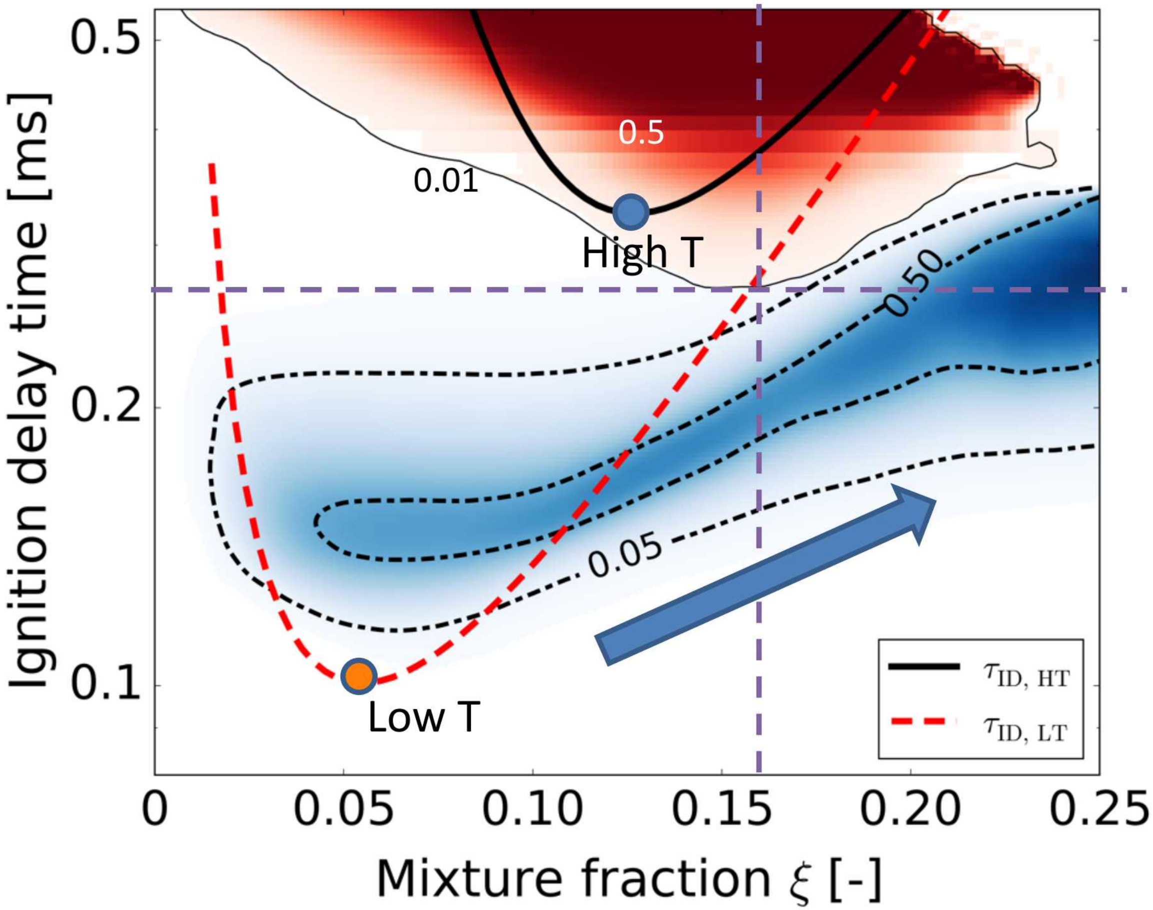


Temporal evolution of selected reactive scalars

Conditional statistics reveal ignition dynamics

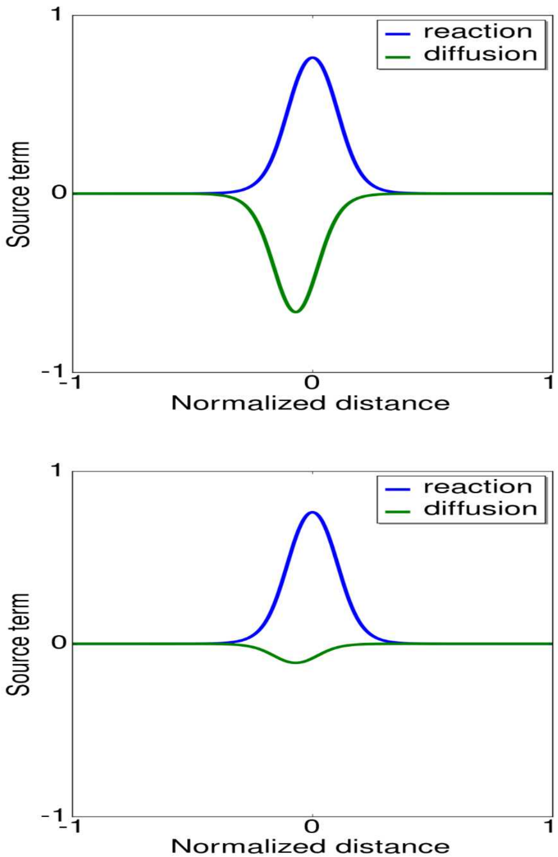


Turbulent versus homogeneous ignition



Low-T and high-T ignition in jet can be faster and than in a PSR !

Propagation mechanism for low-T reaction front



Sketch of reaction / diffusion balance along normal for KET for flame and ignition kernel

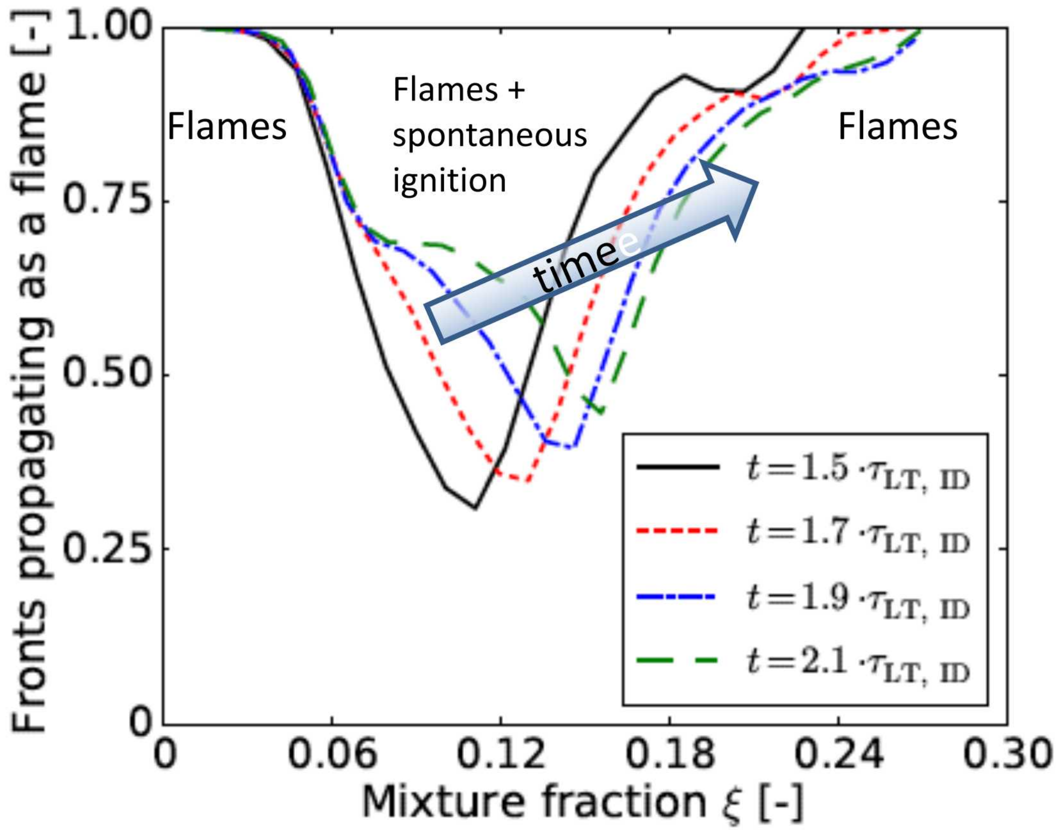
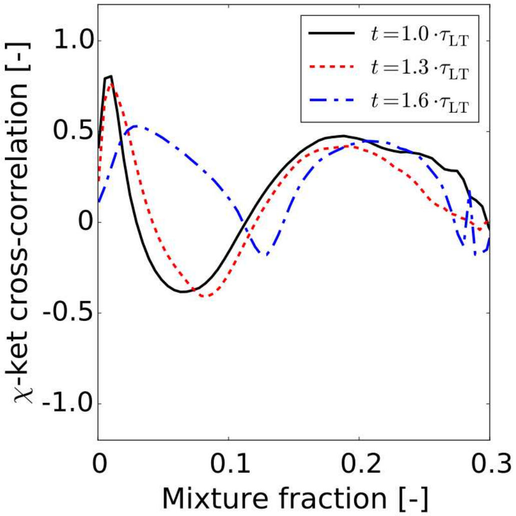
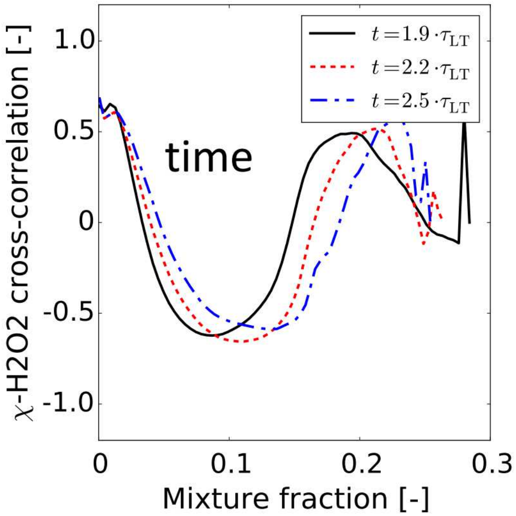


Figure: Fraction of reactive low-T fronts propagating as a flame

Low-T fronts propagate through diffusively supported flame

Effect of Scalar Dissipation Rate on Low Temperature Ignition





Conclusions

- Low-temperature reactions create the conditions for high-temperature ignition to occur faster than under homogeneous conditions;
- Low-temperature front appears to propagate through a diffusively supported cool flame;
- High scalar dissipation appears to delay low-temperature ignition; however, it leads to faster ignition at very rich mixture conditions;
- High-T ignition starts at conditions richer-than-homogeneous conditions (ξ=0.16 compared to ξ=0.12). Edge flames are seen to form around ξ_{st}. High-T flame ignites mainly by propagation of rich premixed flames following hot ignition to ξ_{st}.

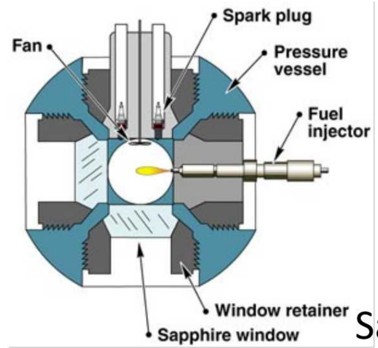
DNS of multi-injection mixing and combustion at compression ignition engine conditions

M. Rieth[a], M. Day[b], C.-B. Kweon[c], Jacob Temme[c]

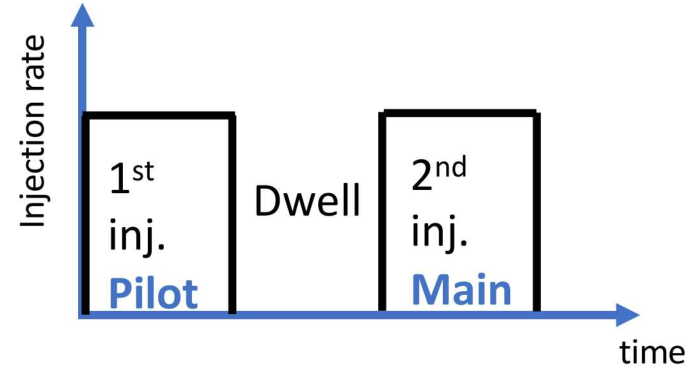
J.B. Bell[b], J.H. Chen[a]

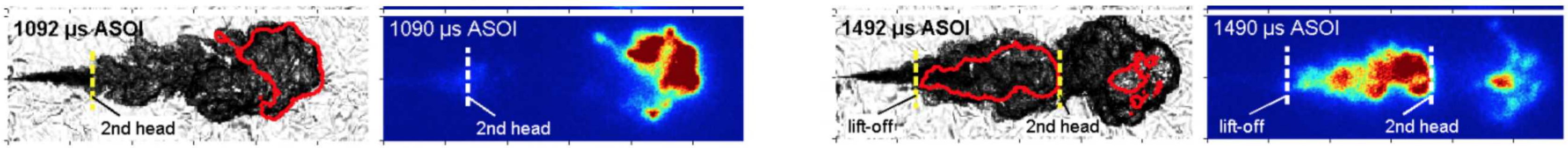
[a]Sandia National Laboratories
[b]Lawrence Berkeley National Laboratory
[c]U.S. Army Research Laboratory

Objectives & Setup



Sandia Spray A experiment[2]





Ignition delay of 2nd injection decreased by roughly factor 2[3]

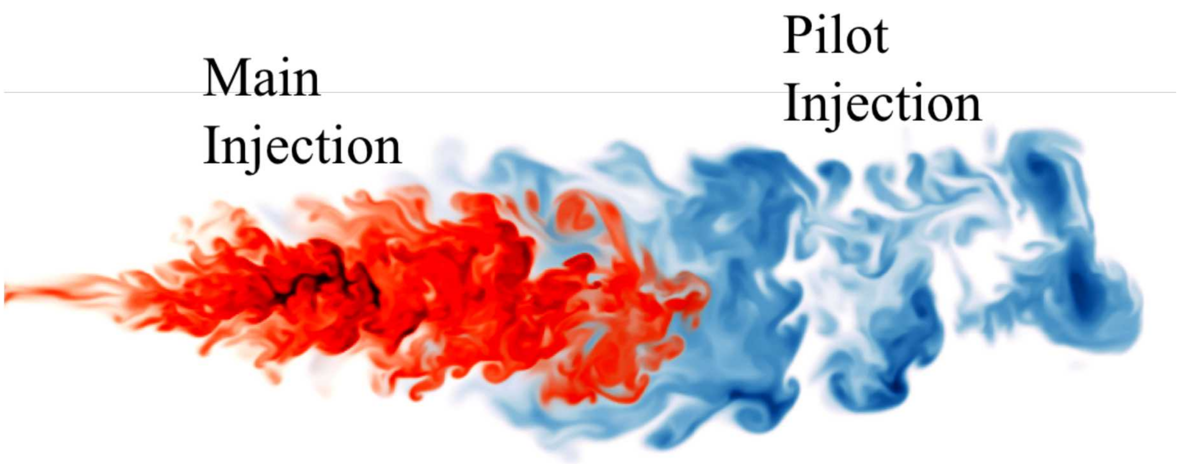
- Purely gaseous n-dodecane/air jet @ T=470K, Z=0.45
- Ambient conditions: 900K, 15% O_2, 85% N_2, 60atm
- Conditions adapted from Dalakoti et al.[1]
  → **downscaled ECN Spray A, keeping Da constant** (Re≈19,000, Da_{jet} ≈0.02)
- Multi-injection: 0.5 ms pilot, 0.5 ms dwell, 0.5 ms main
- **Main injection sees very different conditions compared to pilot injection**
- **How do mixing and different thermo-chemical conditions affect ignition in the main injection?**

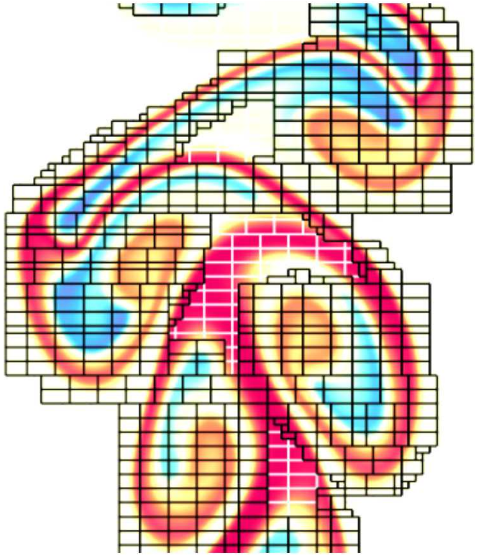
[1]Dalakoti et al., ICDERS, 2017. [2]www.crf.sandia.gov. [3]Skeen et al., JSTOR, 2015.

PeleLM Code & Numerical Setup

- **PeleLM** – low-Mach adaptive mesh refinement code based on AMReX
- Spectral deferred correction scheme for fluid dynamics-chemistry coupling
- Code is open-source at **https://amrex-combustion.github.io/**

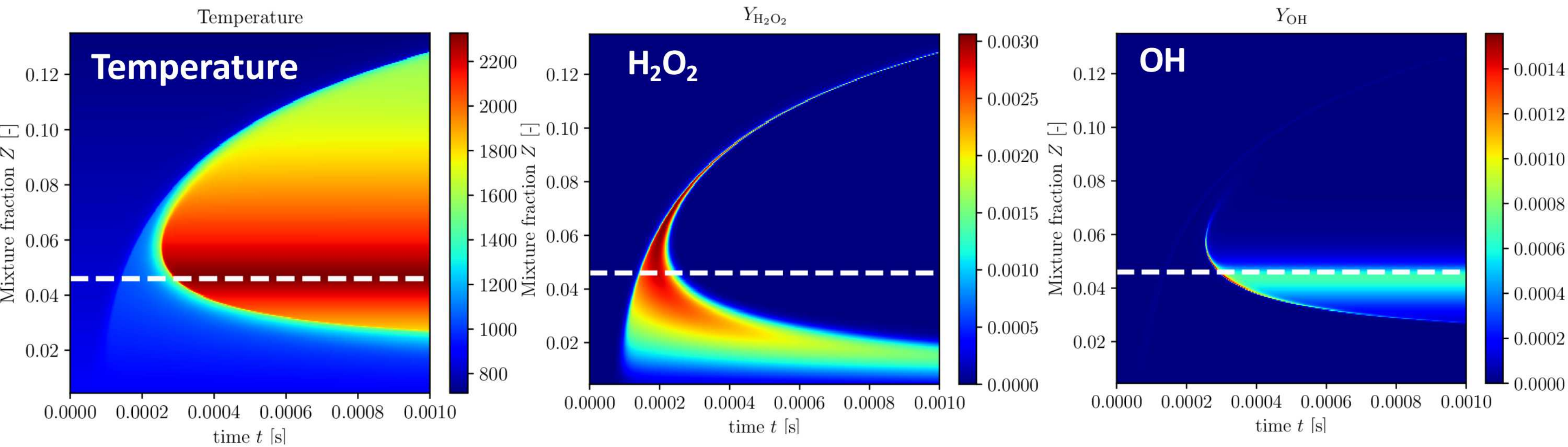
- Resolution ~1.25 micron required for rich premixed cool flames, **currently 5 micron for full multi-injection run**
- Size of simulation: 0.5B cells (O(100)B cells full run without AMR)
- 35 species reduced n-dodecane mechanism (Yao et al., 2017; Borghesi et al., 2018)





Emmett et al., arxiv, 2018.
E. Motheau AMReX gallery.

Zero-dimensional n-dodecane ignition

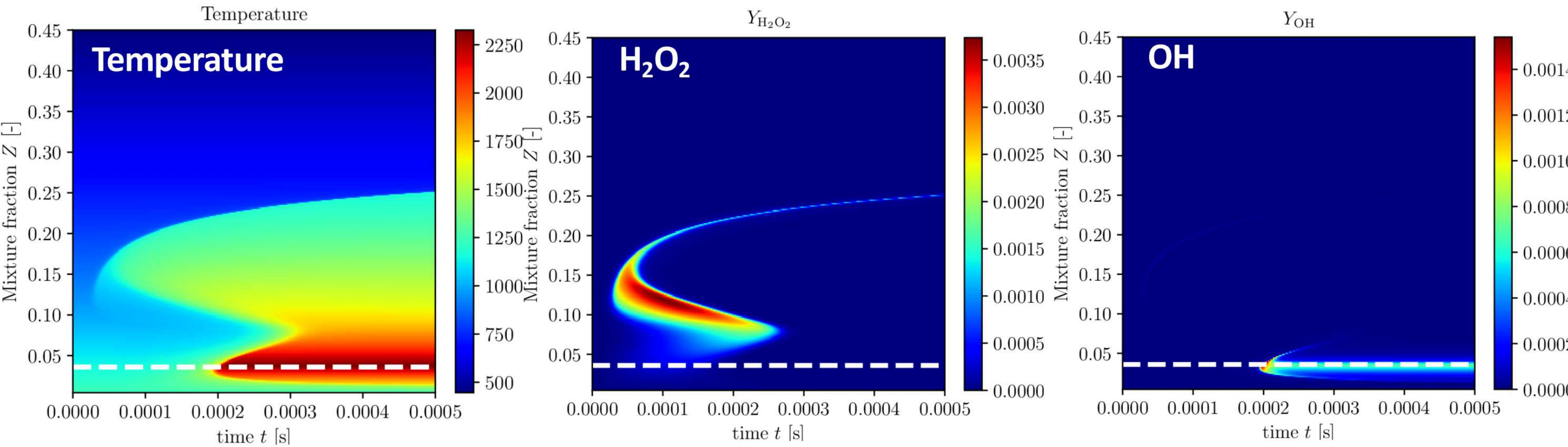


- N-dodecane exhibits two-stage ignition with minimum ignition delay at ‘preferred mixture fraction’ for each stage[1]
  - H_2O_2 is a marker for low temperature combustion
  - OH is a marker for high temperature combustion

[1]Mastorakos, PECS, 2009.

Zero-dimensional n-dodecane ignition with products

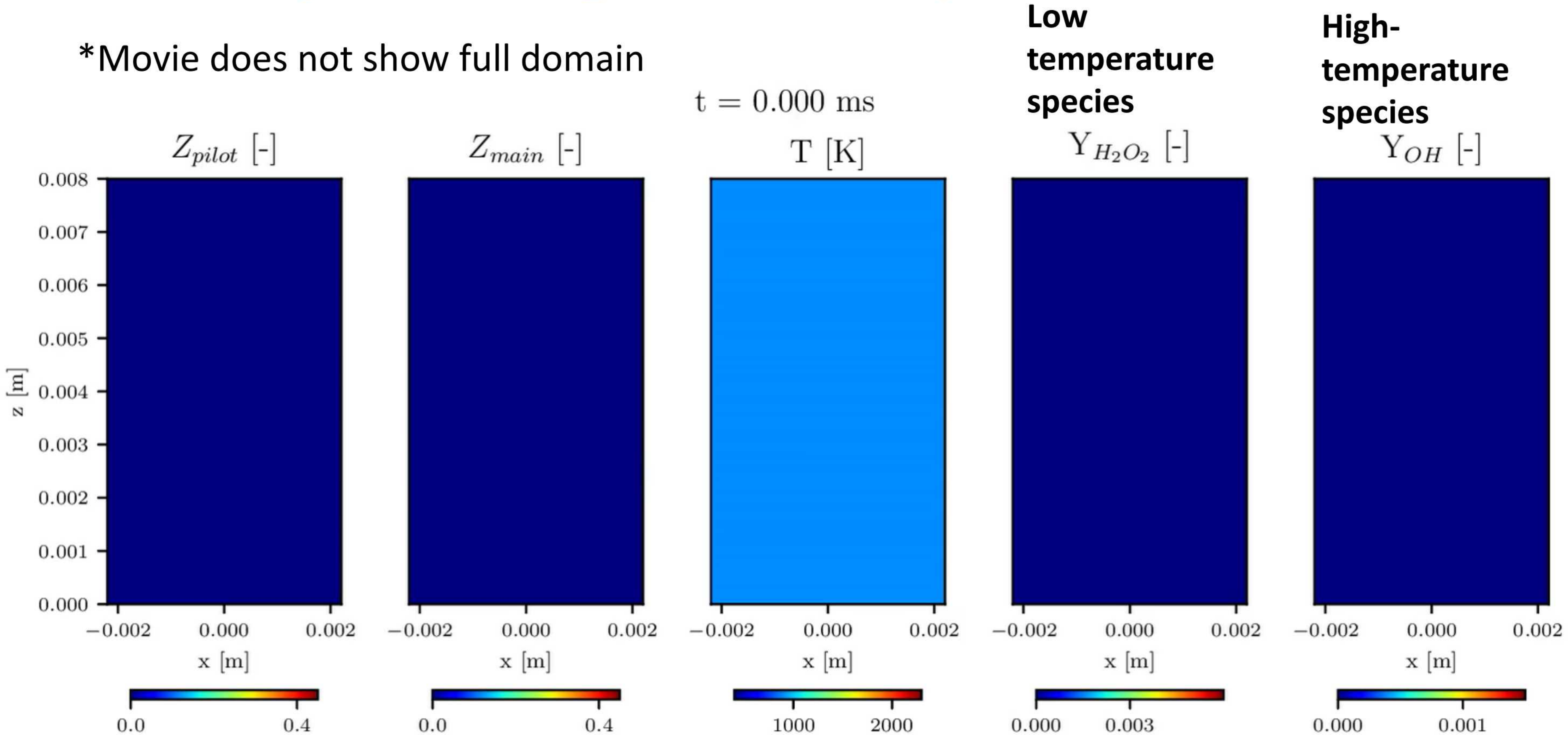
Oxidizer now consists of an equilibrated lean mixture with Z=0.01



- Low temperature ignition shifts toward richer mixtures (by almost a factor of 3, has a much shorter ignition delay while hot ignition remains the same)

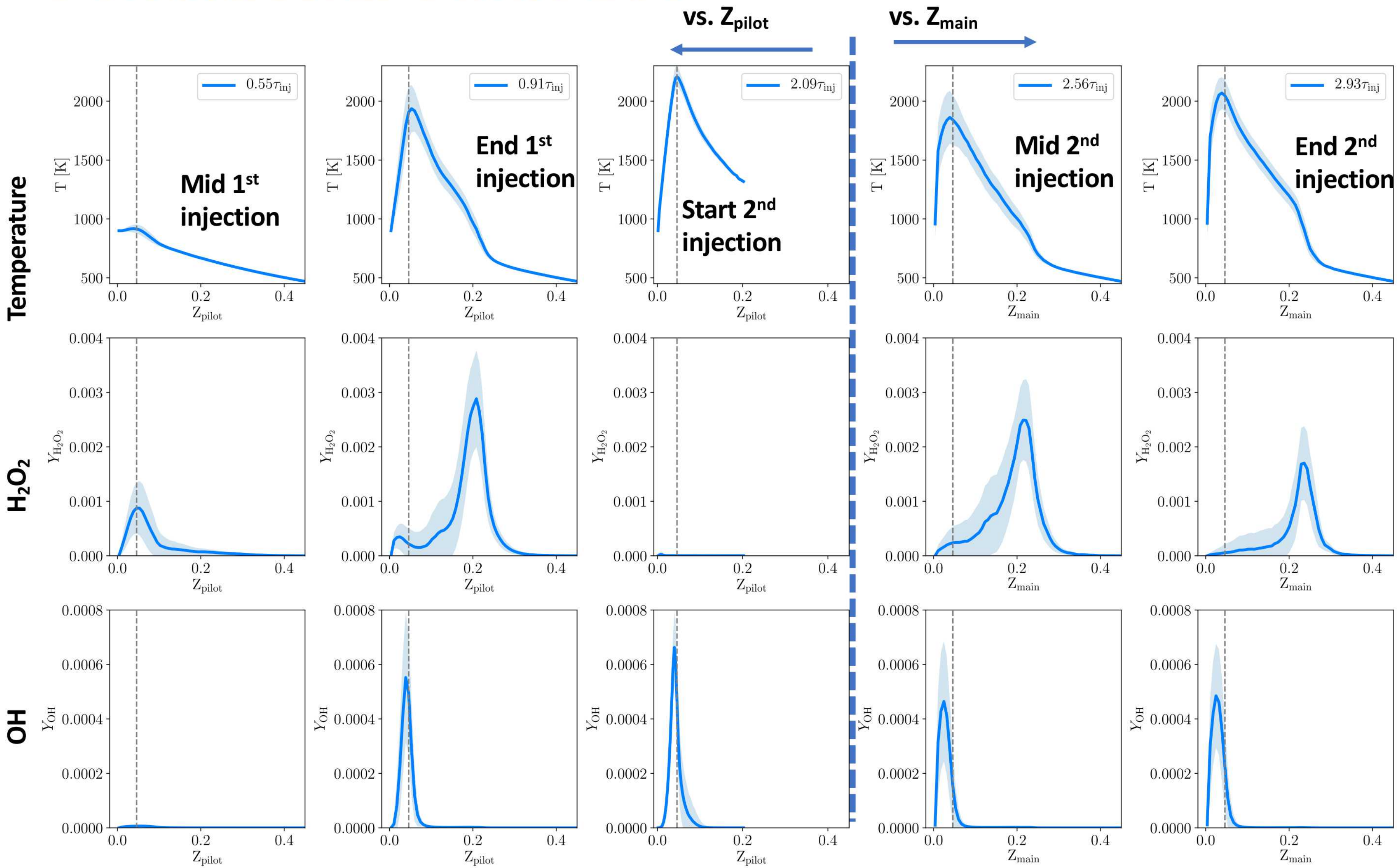
Multi-injection ignition sequence

*Movie does not show full domain

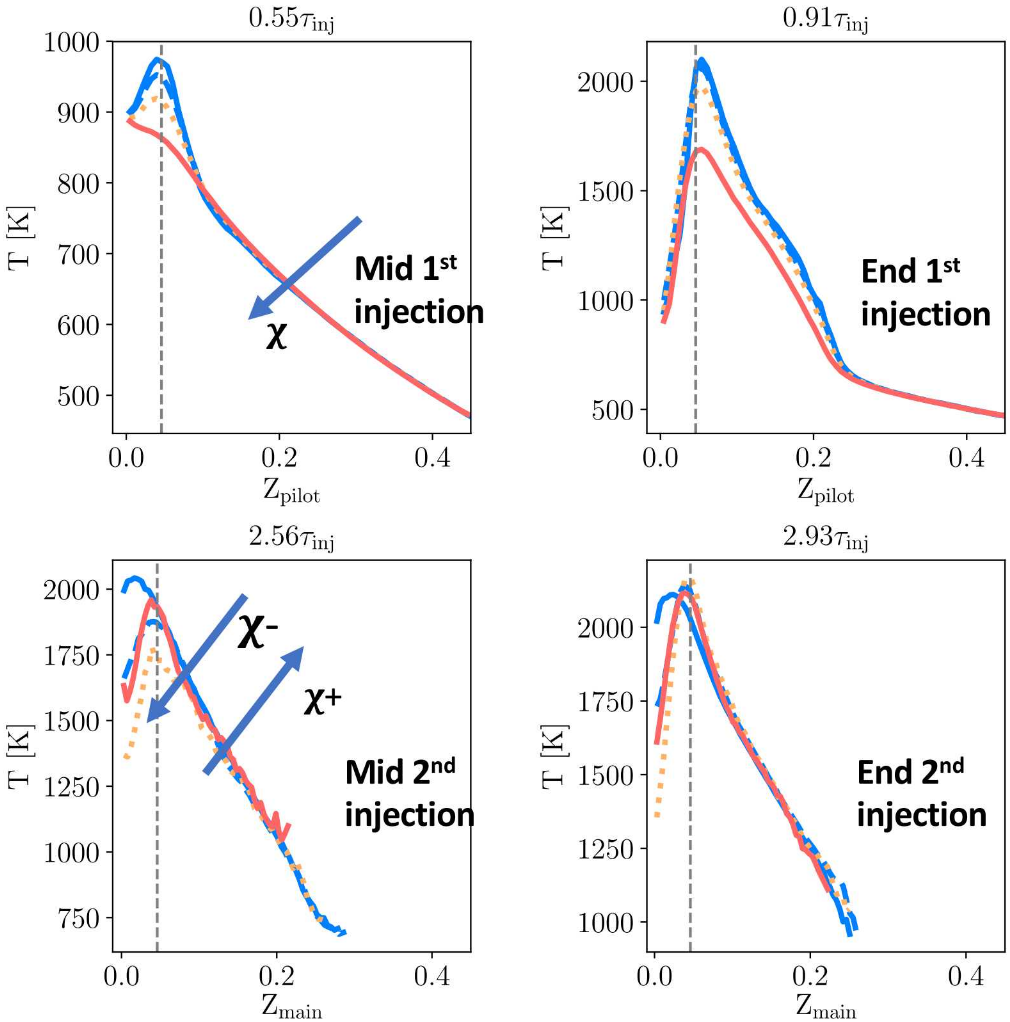


Mixture fractions track fluid from individual injections (two additional transport equations)

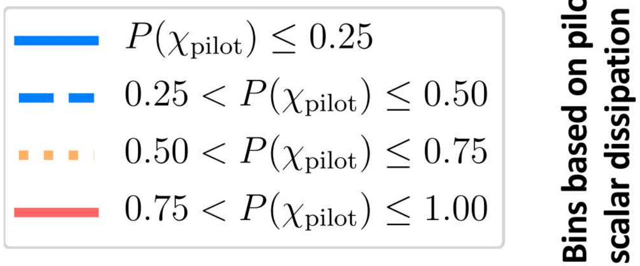
Conditional statistics



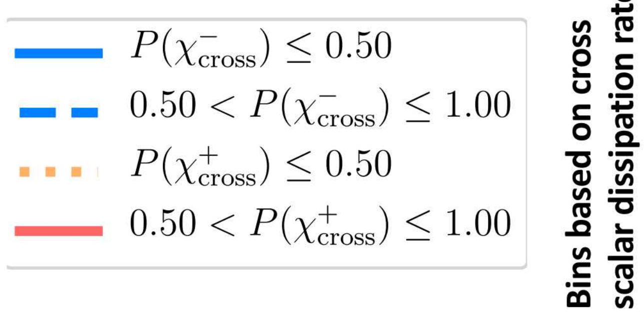
Effect of mixing on ignition



$$\chi_{\mathrm{pilot}} = 2D(\partial Z_{\mathrm{pilot}}/\partial x_j)^2$$

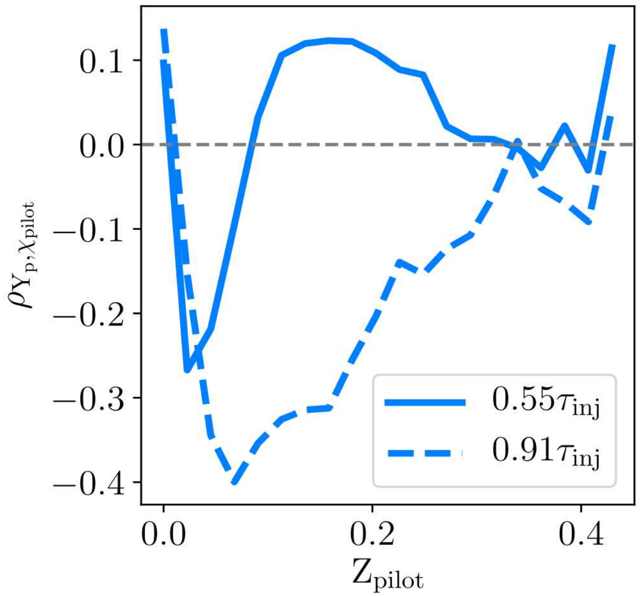


$$\chi_{\mathrm{cross}} = 2D(\partial Z_{\mathrm{pilot}}/\partial x_j \cdot \partial Z_{\mathrm{main}}/\partial x_j)$$

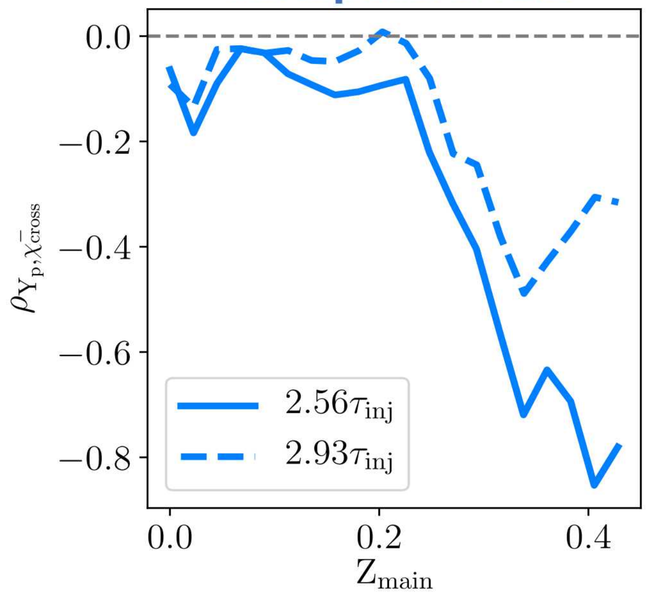


Effect of mixing on ignition

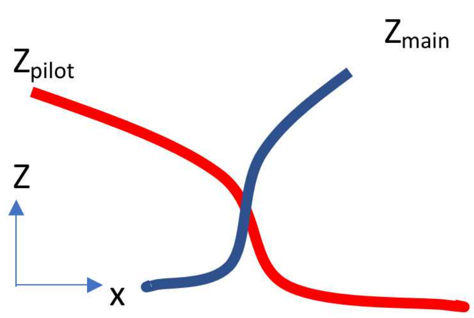
1st injection
Correlation between progress variable and pilot scalar dissipation rate



2nd injection
Correlation between progress variable and cross scalar dissipation rate



Only negative values of cross scalar dissipation rate taken into account



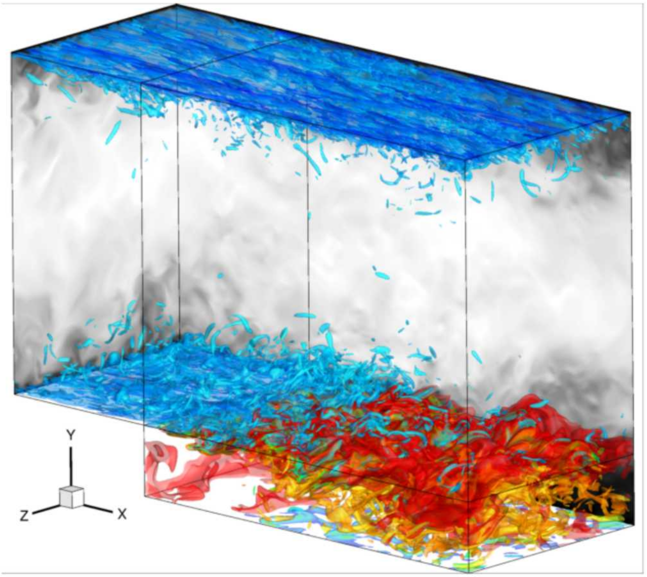
1st injection consistent to work by Borghesi et al., C&F, 2018.

Conclusions

- First- and second stage pilot ignition consistent with previous numerical studies
- Accelerated ignition for main injection observed consistent with experiments
- Pilot/main mixture fraction scalar dissipation rates show similar log-normal-like pdfs
- Cross SDR pdf has sharp peak and stretched exponential tails, skewed toward negative values
- **Strong mixing inhibits ignition of first injection, promotes ignition of second injection**

DNS of a turbulent premixed flame stabilized over a backward facing step

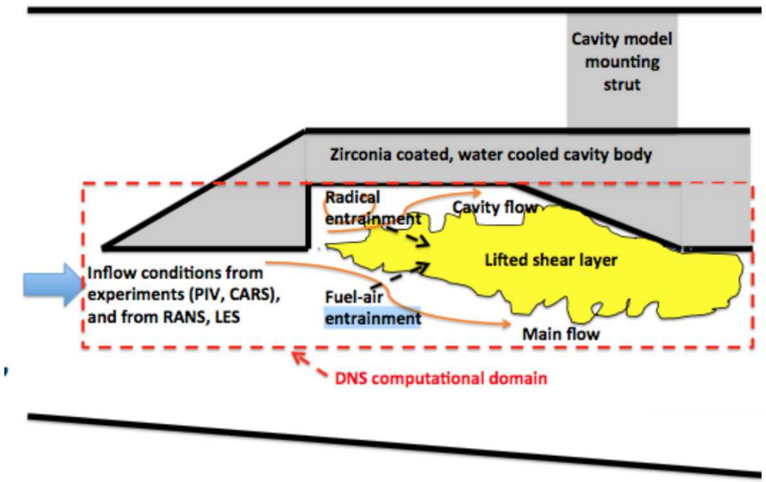
Konduri Aditya, Hemanth Kolla and Jacqueline H. Chen
Sandia National Laboratories

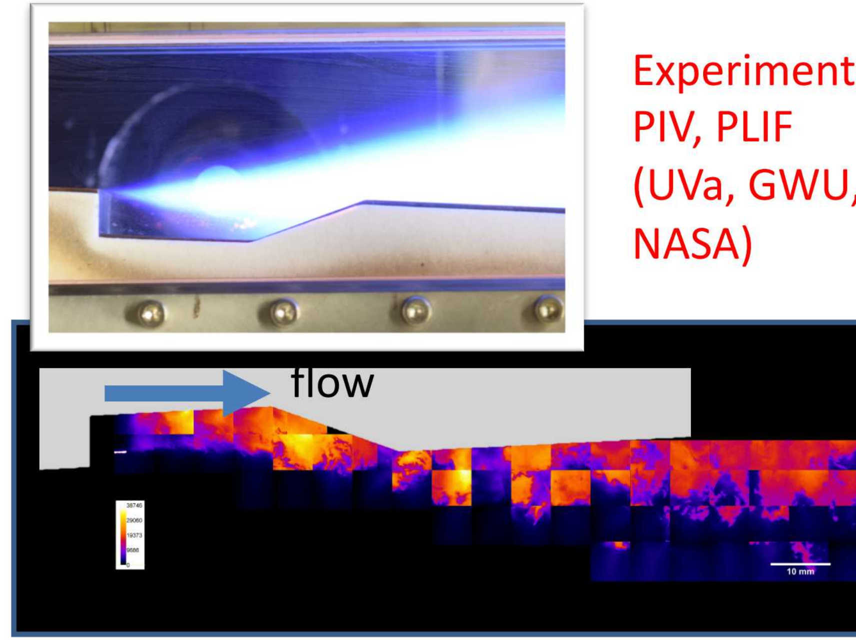


Sandia National Laboratories

Acknowledgements:
ASCR, Office of Science, DOE
OLCF, NERSC

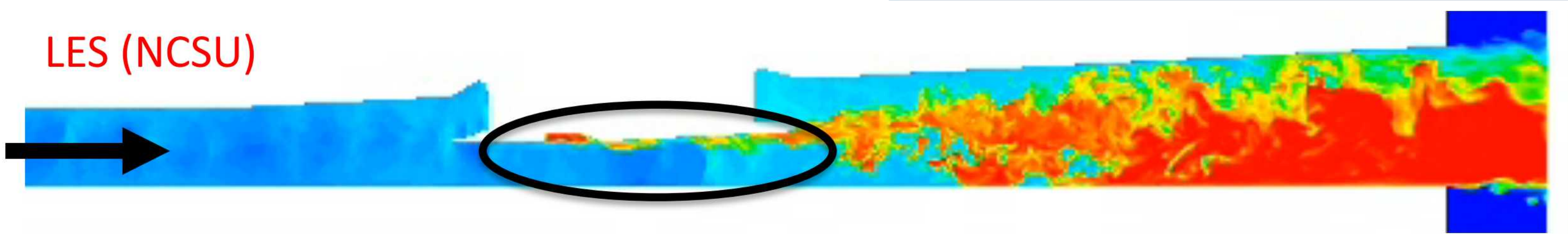
Overview





Experiments PIV, PLIF (UVa, GWU, NASA)

LES (NCSU)

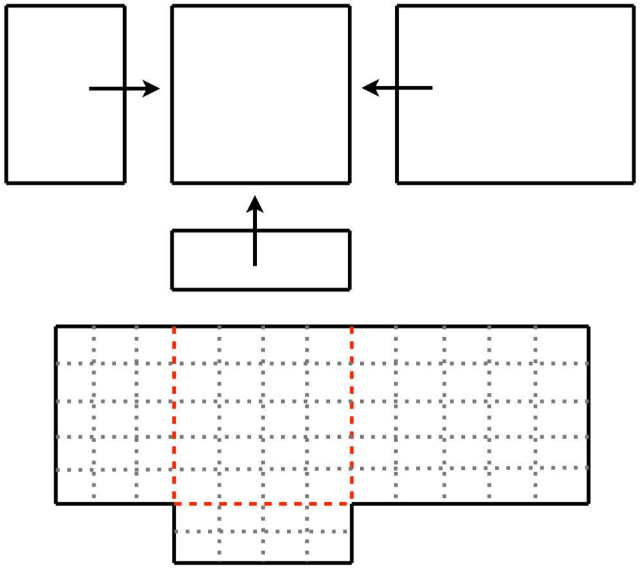


Gain insights into:

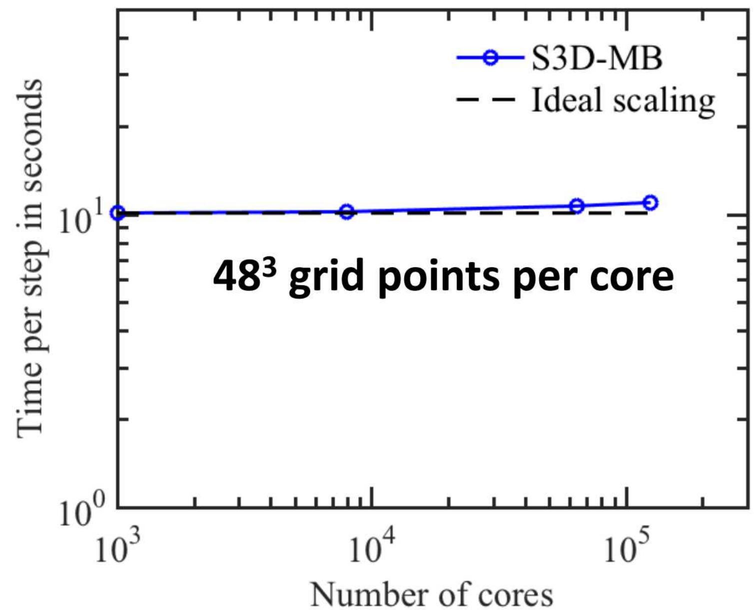
- Flame stabilization mechanism
- Effect of heat release
- Turbulence and chemistry interactions

S3D - Multiblock

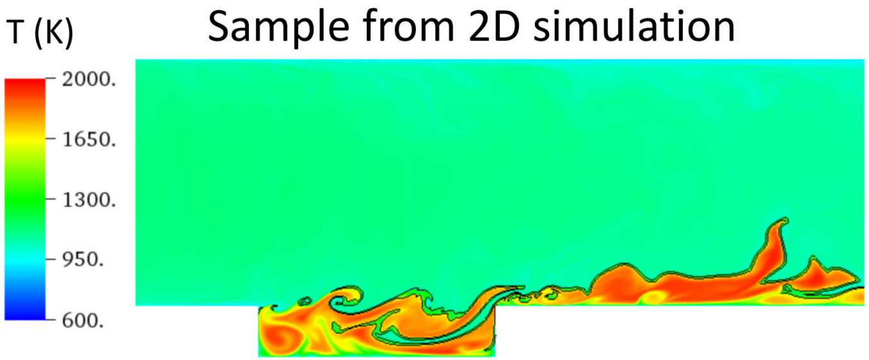
Multiblock construction



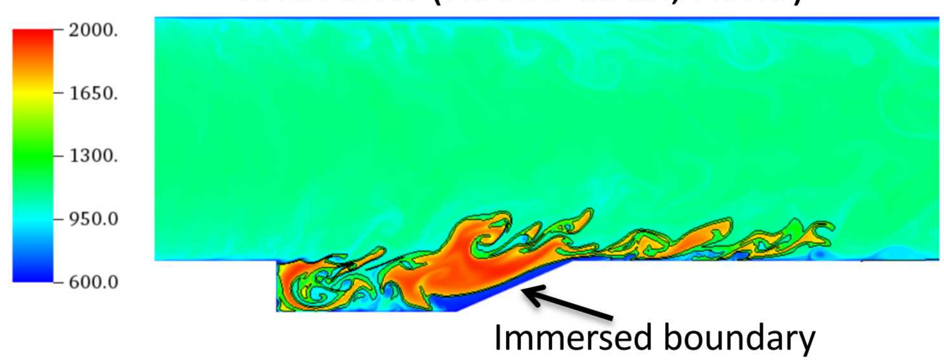
Weak scaling on Titan



Sample from 2D simulation

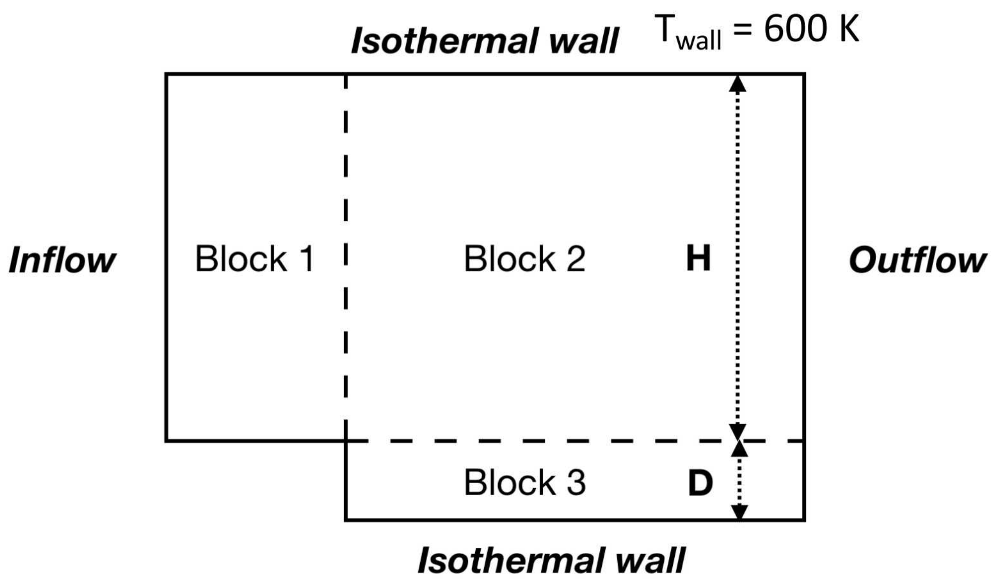


With IBM (Rauch et al., 2018)



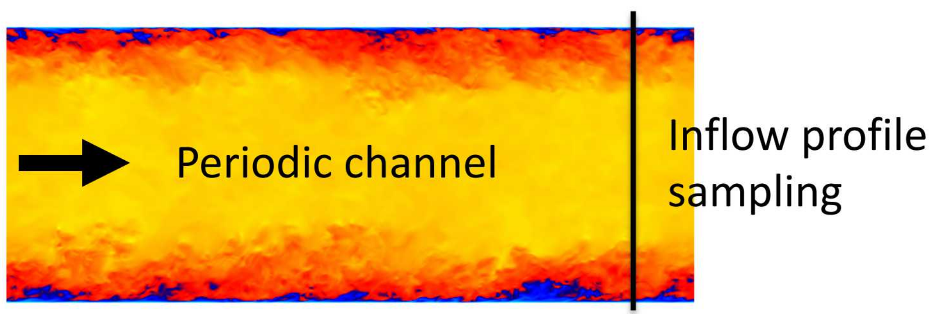
Backward-facing step

Ethylene-air
$\Phi = 0.42$
$U = 200$ m/s
$u' = 10\%$
$T = 1125$ K



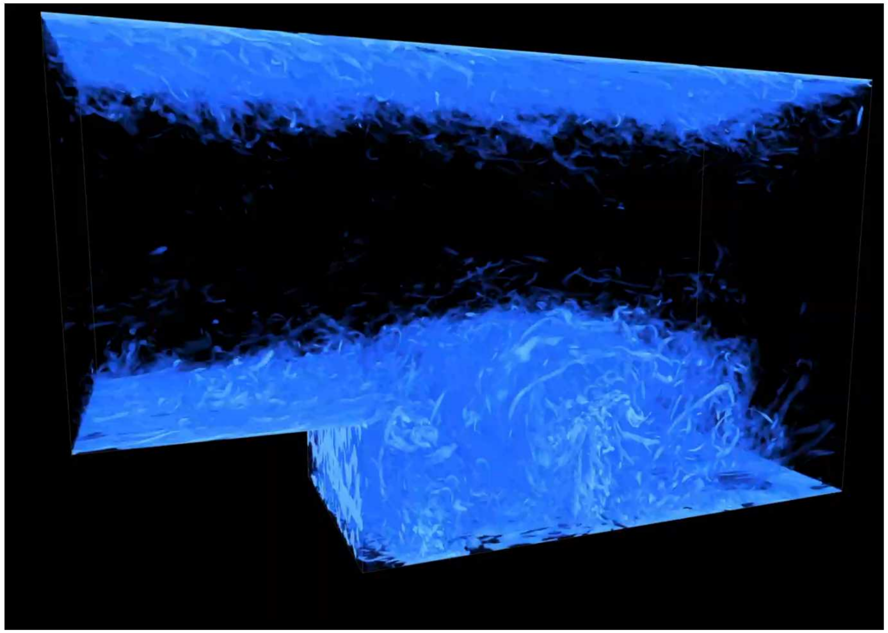
H	1.47 cm
D	0.3048 cm
Re_H	35000
Re_T	788
Grid count	2.6 billion
CPU hrs	25 million

- **Mechanism:** 22 species non-stiff reduced ethylene-air (Lu et al. 2012)
- **Transport model:** mixture averaged
- **Turbulent inflow profile:** feed data generated from a separate 3D DNS of channel

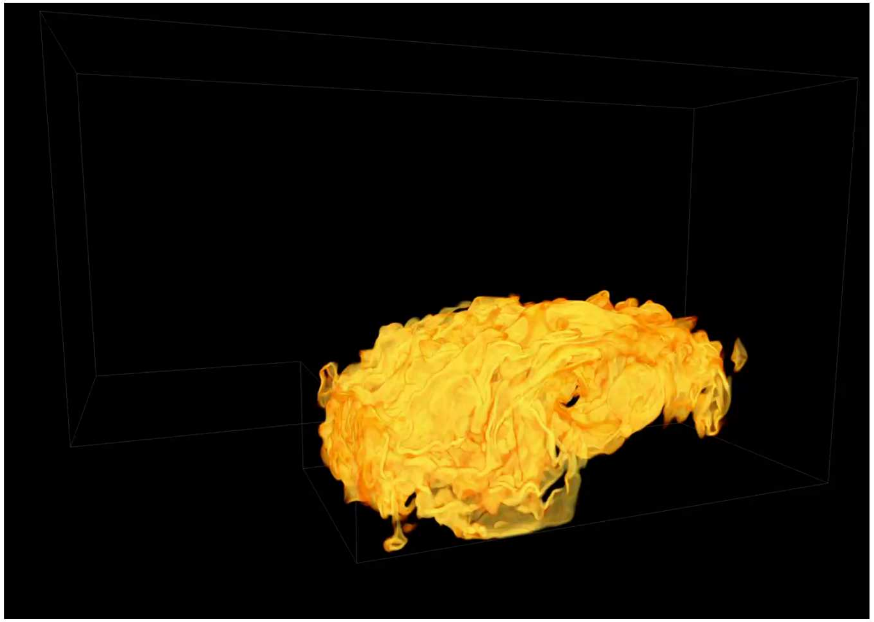


Flame stabilization

Vorticity magnitude

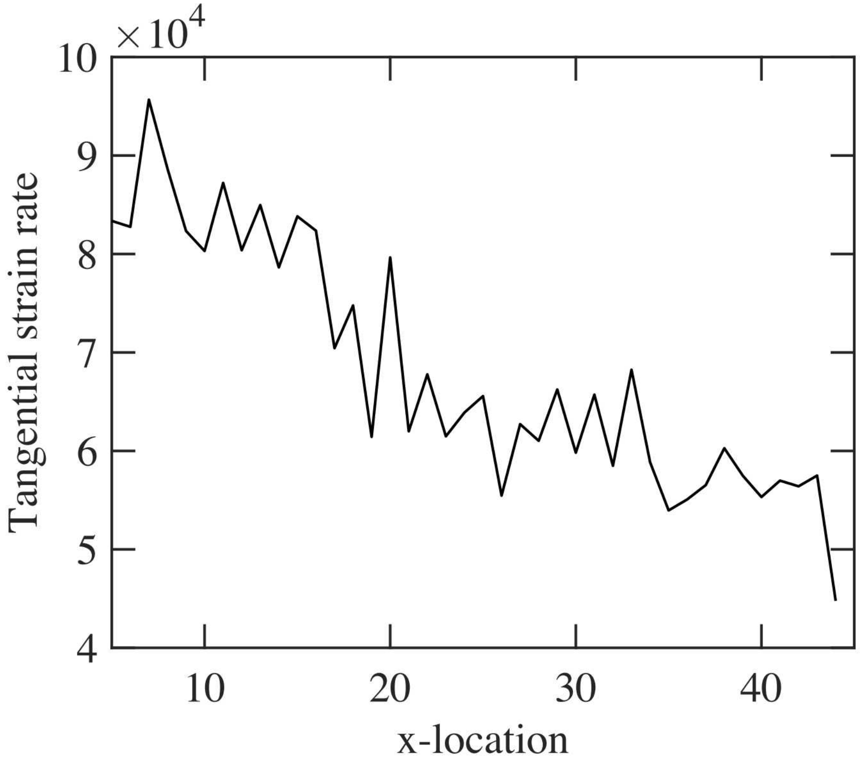


Heat release rate



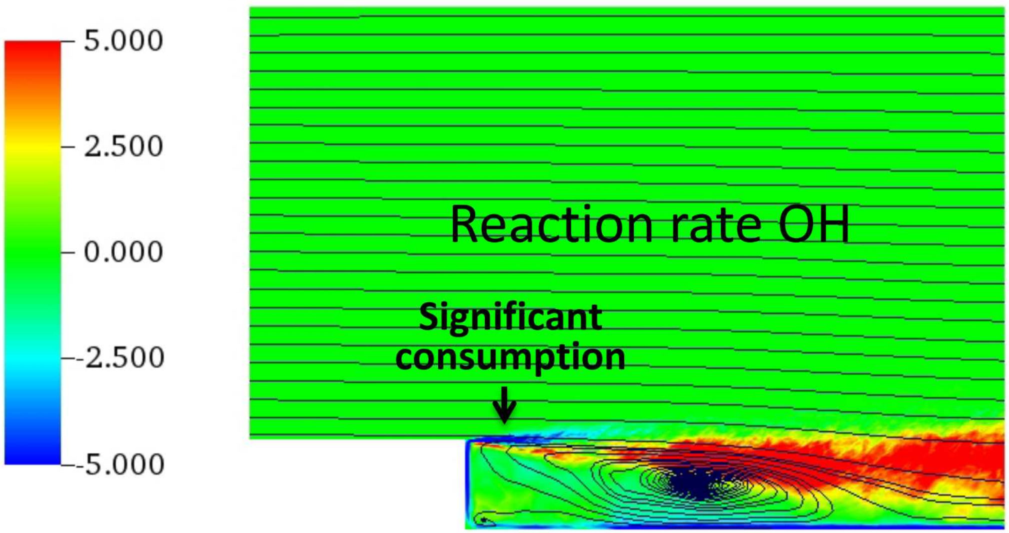
- Flame stabilizes near the corner of the step
- Extends downstream in the shear layer
- Flame inhibits rapid expansion of the channel flow

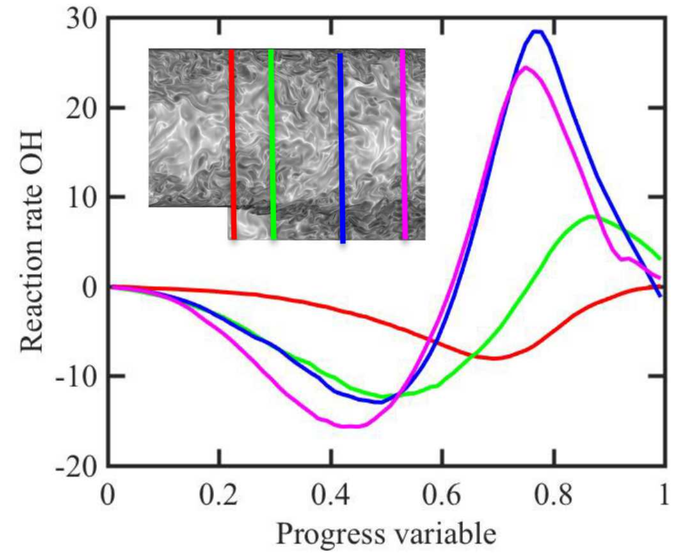
Flame - tangential strain rate

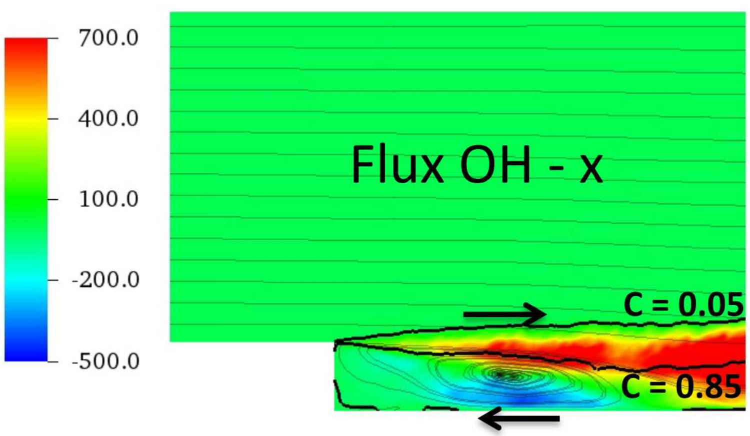


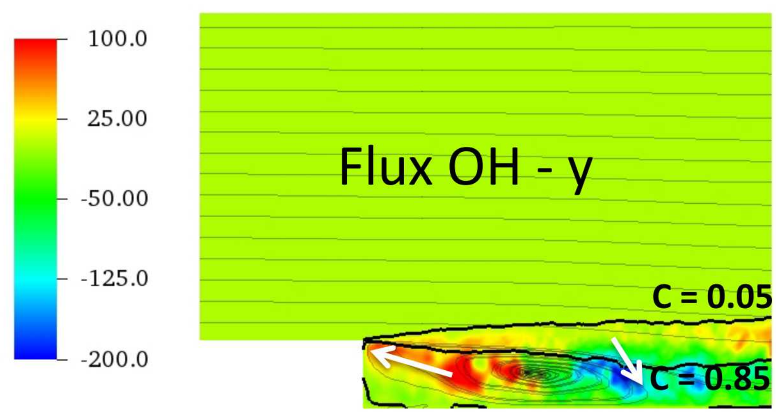
- Strain rate relaxes downstream
- Affects flame structure

Flame stabilization

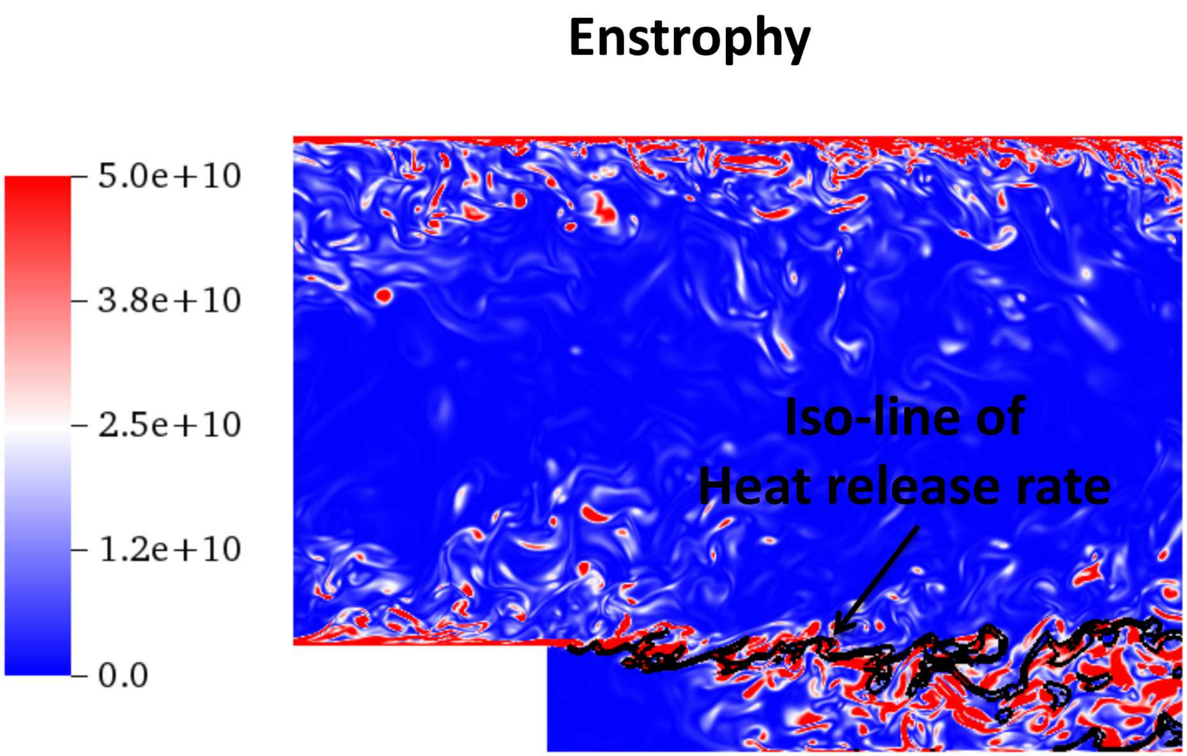






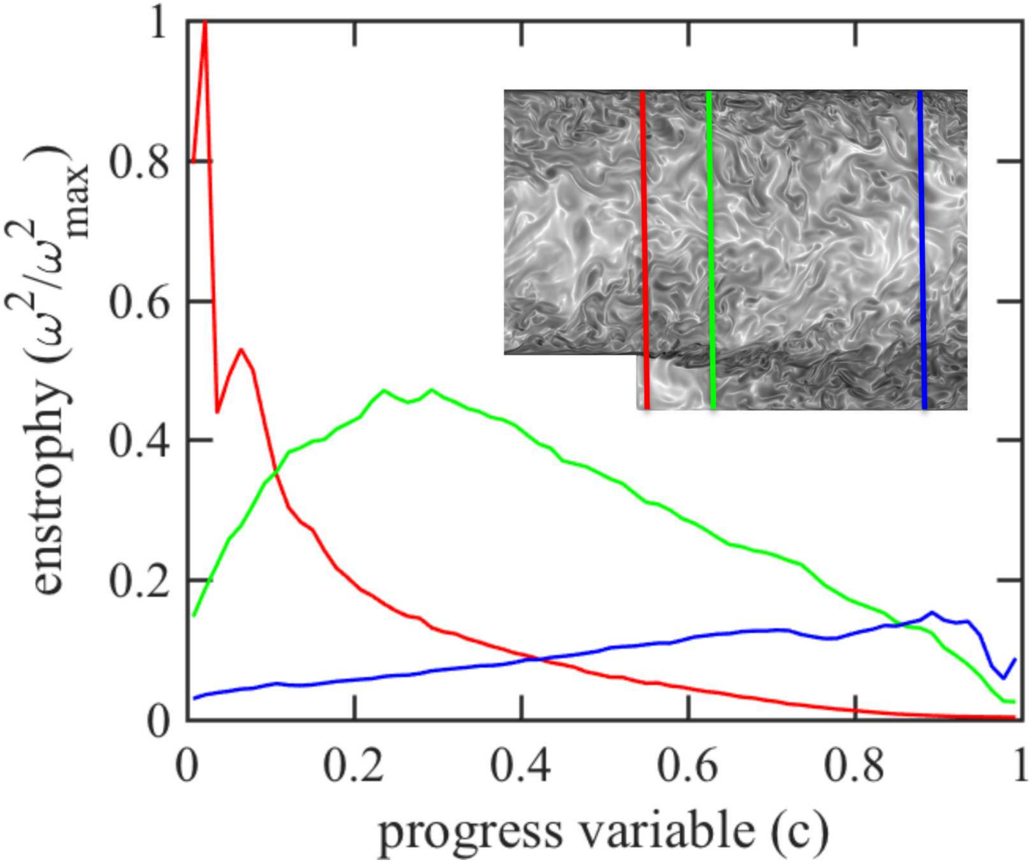


Vorticity dynamics



- Closer to the step: near-wall structures present on the reactant side
- Downstream: significant vorticity present on the product side

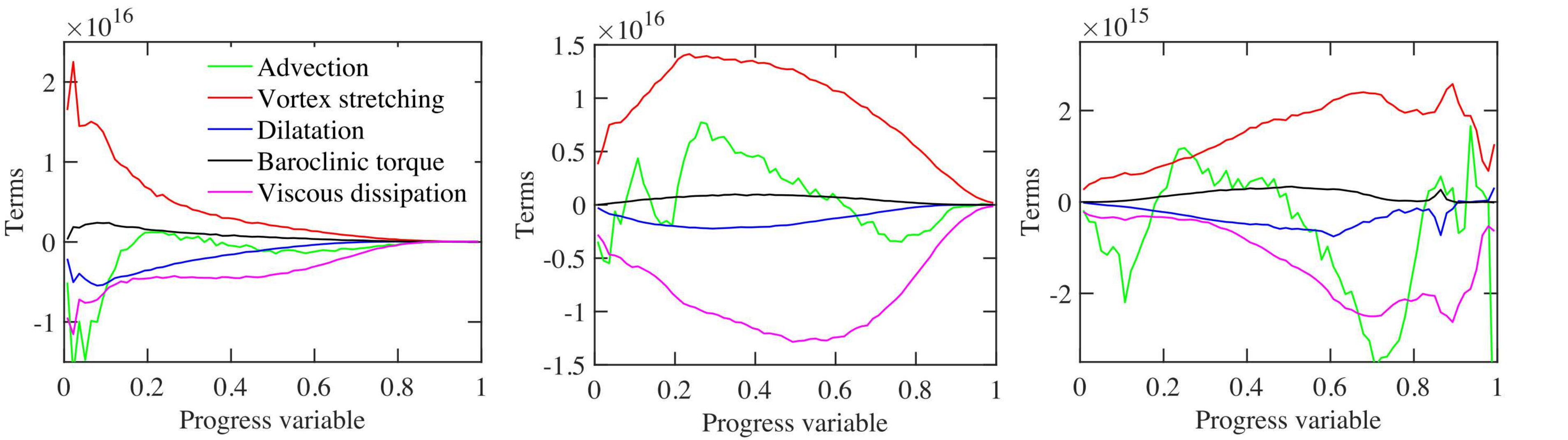
Vorticity dynamics



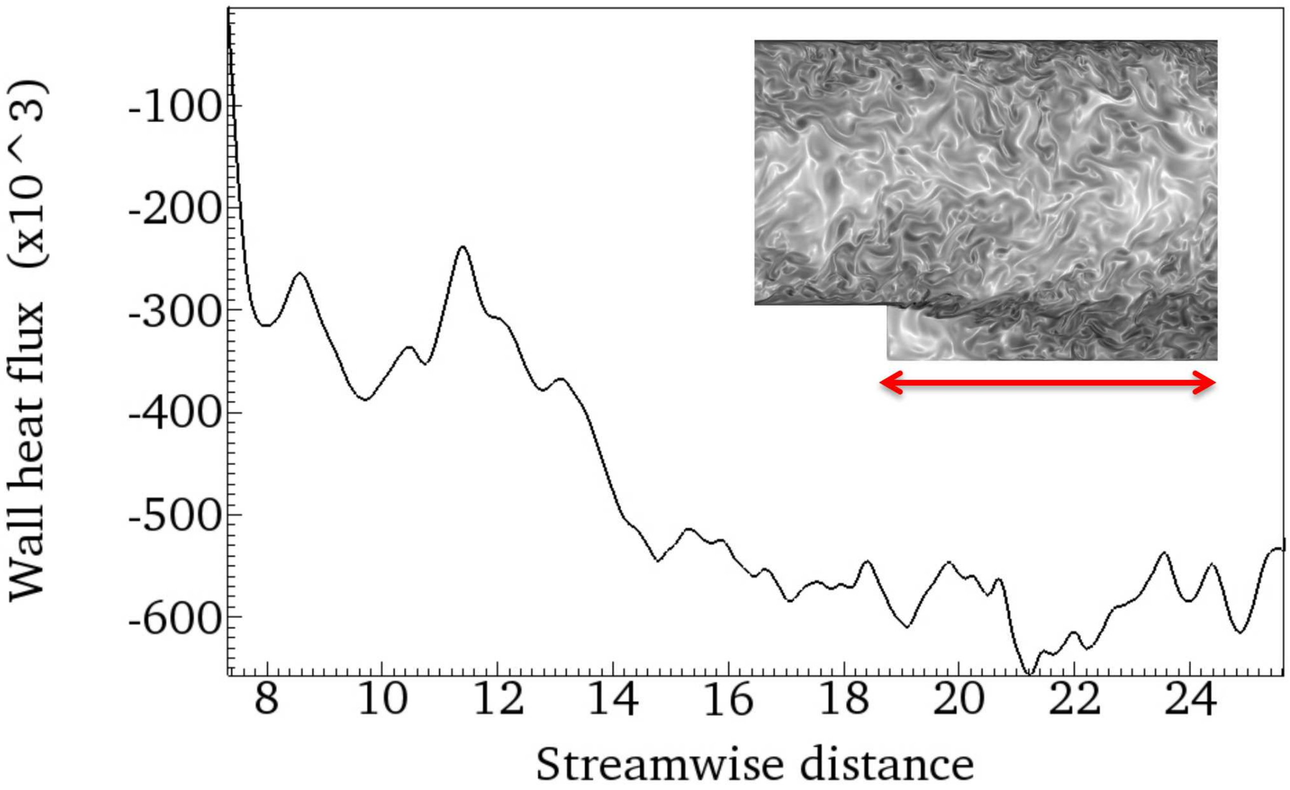
Enstrophy balance shows advection, vortex stretching and viscous dissipation are dominant

$$\frac{\partial}{\partial t}\left(\frac{\omega^2}{2}\right)+u_i\frac{\partial}{\partial x_i}\left(\frac{\omega^2}{2}\right)=\omega_i\omega_j\frac{\partial u_i}{\partial x_j}-\omega^2\frac{\partial u_j}{\partial x_j}+\frac{\omega_i}{\rho^2}\varepsilon_{ijk}\frac{\partial \rho}{\partial x_j}\frac{\partial P}{\partial x_k}+\omega_i\varepsilon_{ijk}\frac{\partial}{\partial x_j}\left(\frac{1}{\rho}\frac{\partial \tau_{kl}}{\partial x_l}\right)$$

Advection | Vortex stretching | Dilatation | Baroclinic torque | Dissipation



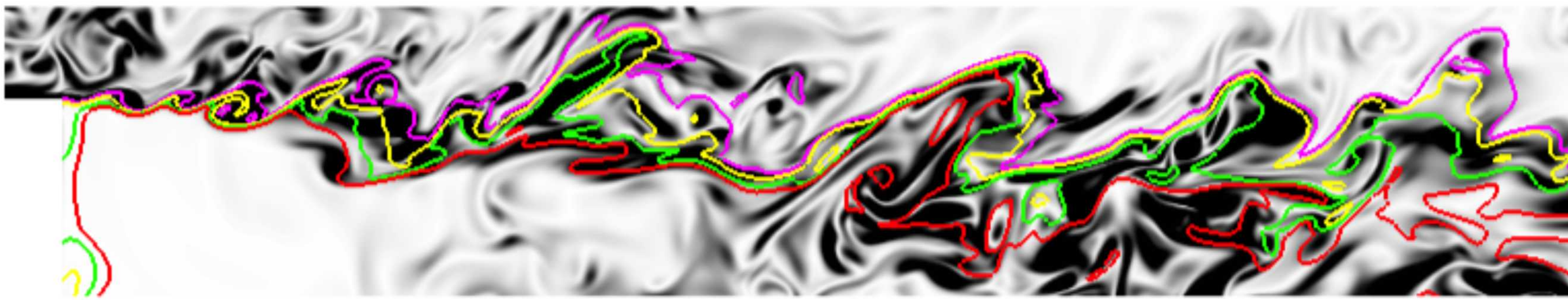
Increased wall heat flux downstream



Flame structure

Grey scale: enstrophy

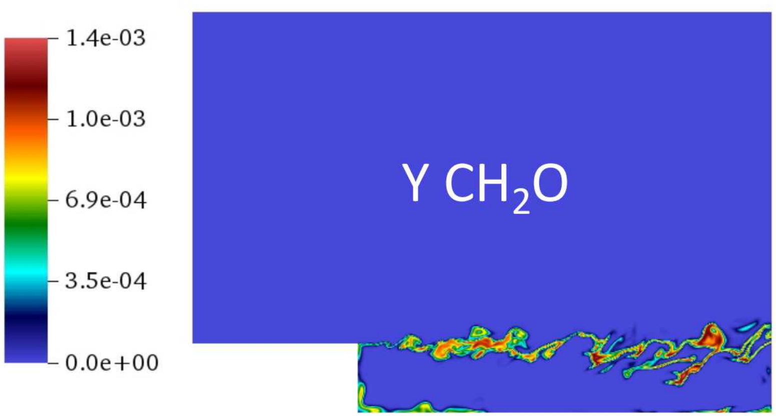
c = 0.2 0.5 0.8 0.9

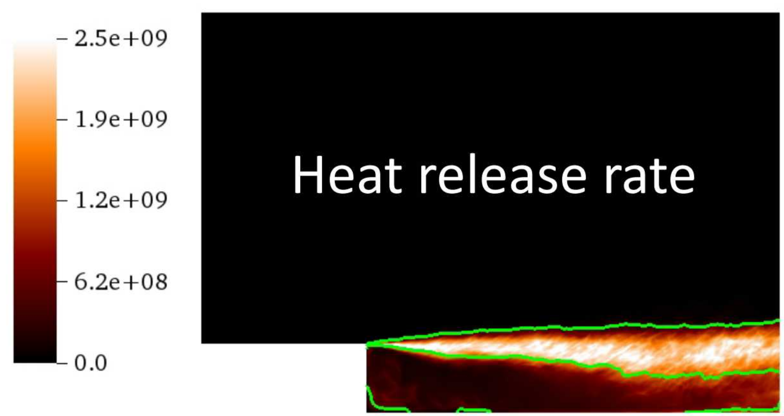


Affects preheat zone

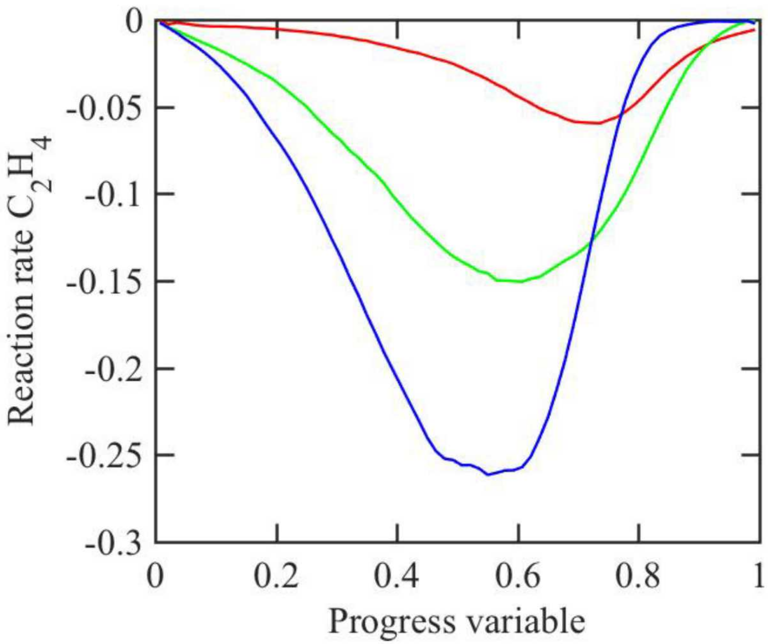
Affects oxidation layer

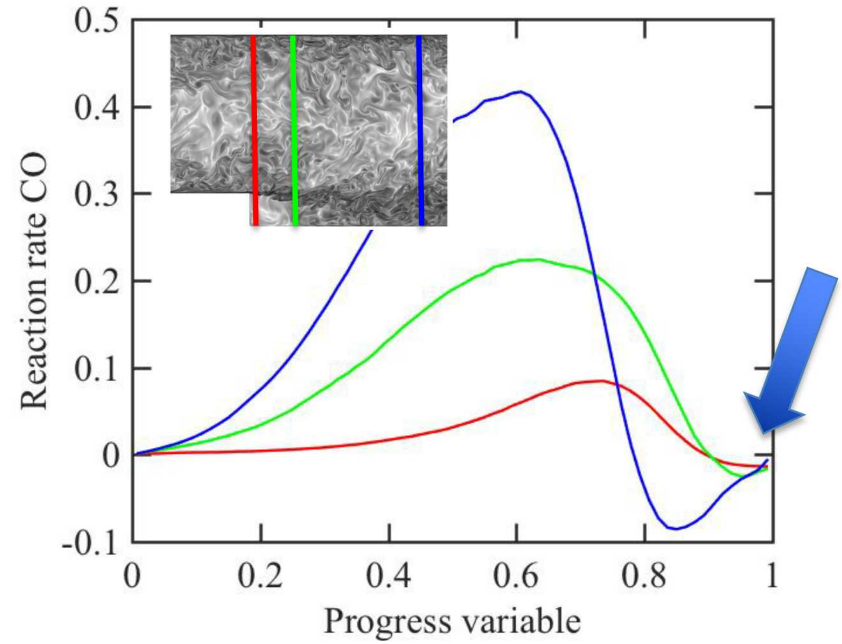
Flame-flame interaction





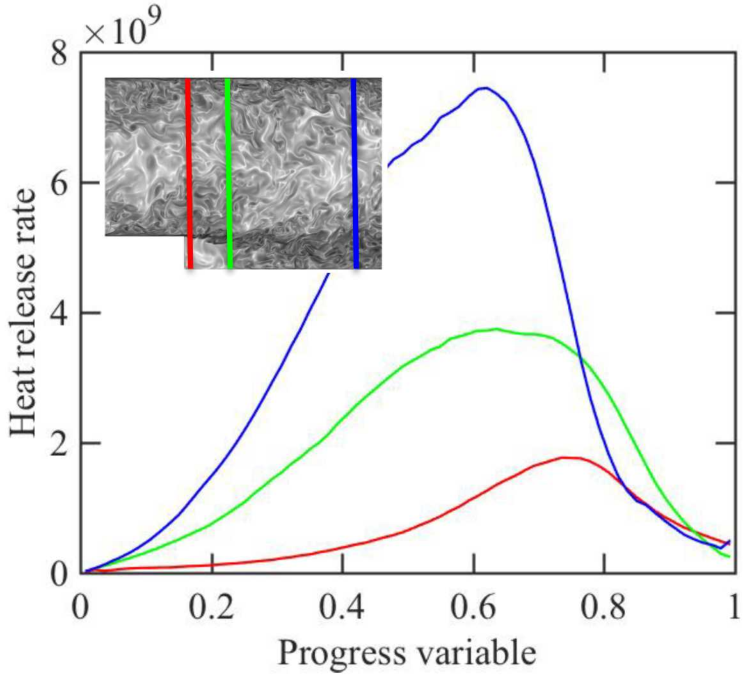
Flame structure

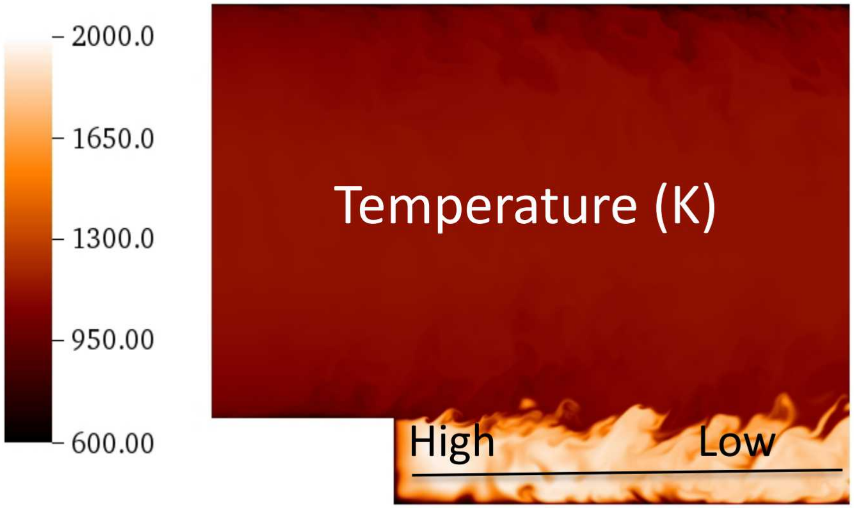




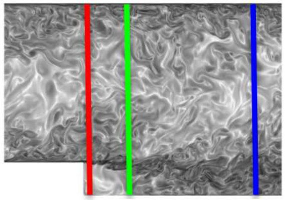
- Due to the high strain rate near the step, fuel is consumed at high progress variable as the flame is pushed into the products (Libby & Williams)
- CO and H2 consumption quenched near the step

Flame structure

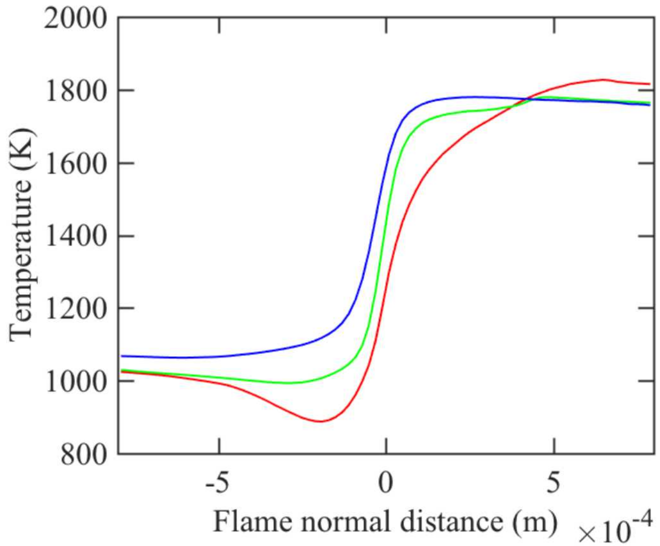


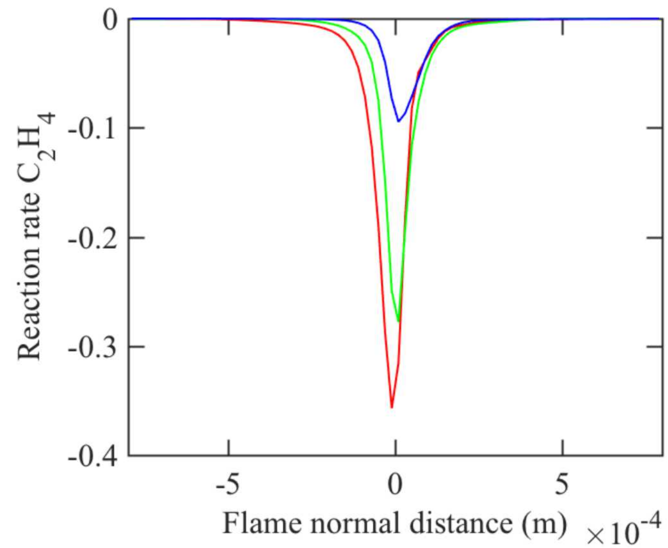


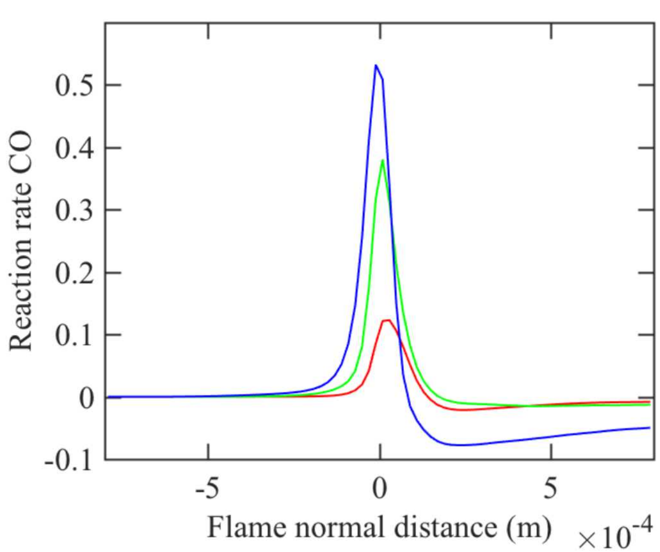
- Heat release rate increases downstream and occurs at intermediate progress variable
- Temperature decreases downstream, due to enhanced mixing in the products

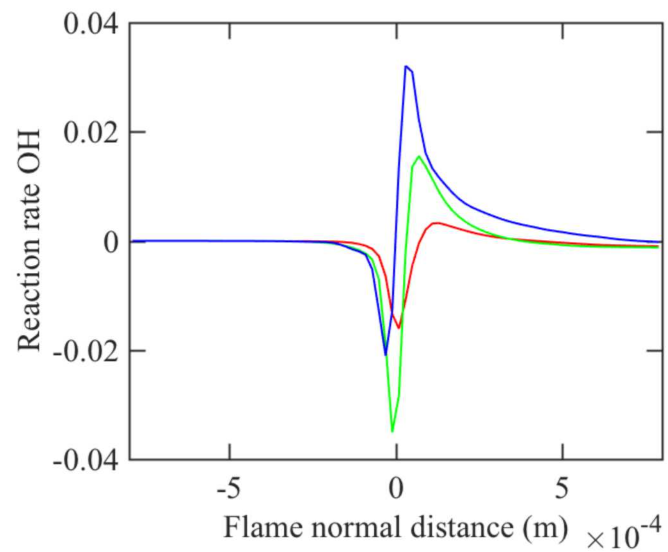


Flame normal statistics









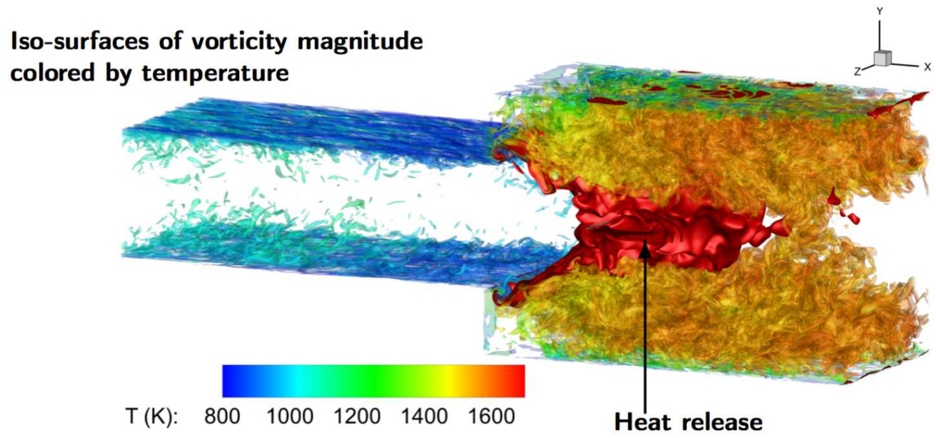
Conclusions

- DNS of C2H4/air flame stabilization behind a backwards facing step
- Strong interaction between recirculation zone, shear layer, and flame brush
- Radicals from the recirculation zone assist in anchoring the flame
- Turbulence generated near-wall migrates towards products downstream of the stabilization point
- Turbulence affects the flame structure and heat losses to the wall

Direct Numerical Simulation of flame stabilization assisted by auto-ignition at *reheat* conditions

Konduri Aditya[a], Andrea Gruber[b], Mirko Bothien[c] and Jacqueline H. Chen[a]

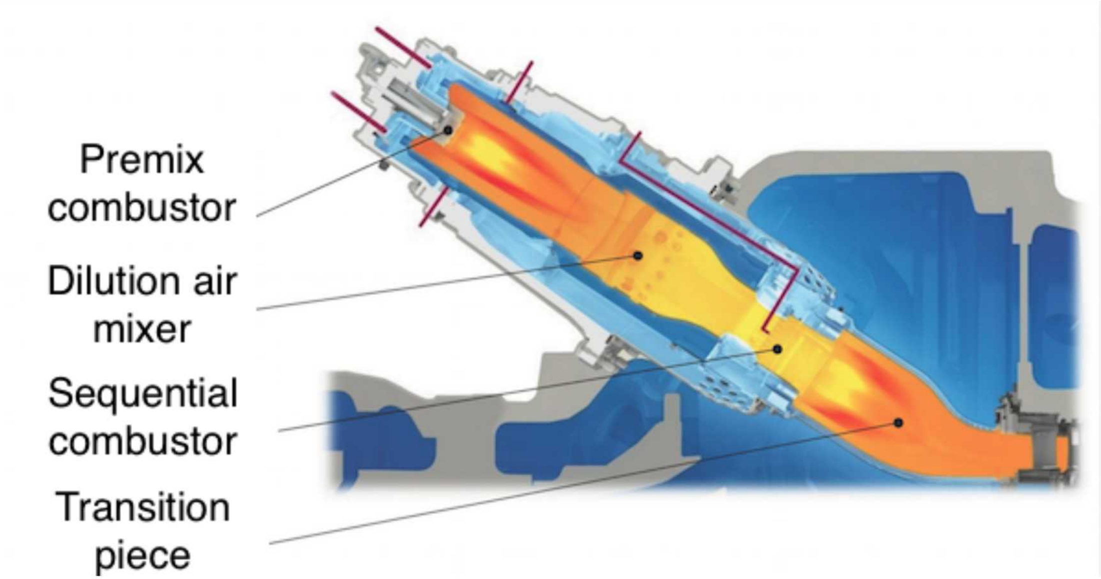
[a]Combustion Research Facility, Sandia National Laboratories, Livermore, CA, USA
[b]SINTEF Energy Research, Trondheim, Norway
[c]Ansaldo Energia, Baden, Switzerland



Acknowledgements:
Basic Energy Sciences, Office of Science, DOE
OLCF, NERSC, Norwegian CCS Research Centre (NCCS)

Aditya et al. PCI 2018

Staged gas turbine combustion



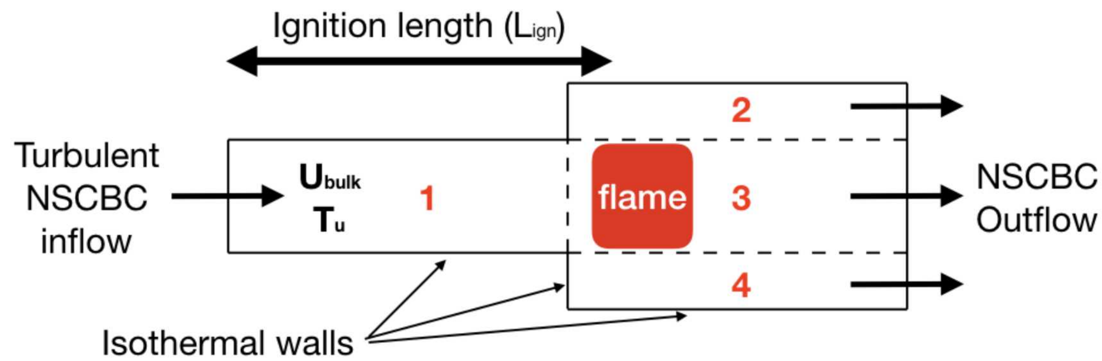
- Originally developed by ABB for high efficiency, load flexibility and low emissions
- Recently improved and simplified (reduced cost) for the H-class GT36
- First (premix) combustion stage based on flame propagation
- Second (sequential) combustion stage based on auto-ignition

Reheat burner

DNS of idealized reheat burner configuration from Ansaldo Energia

Operating conditions:

- Inlet temperature: ~ 1100 K
- Pressure: ~ 20 atm



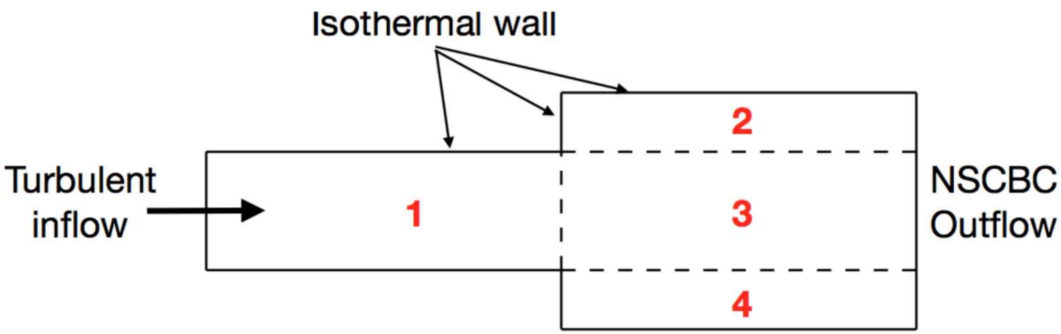
Scaled conditions:

- Mean inlet temperature:
- Pressure: 1 atm
- Fuel: hydrogen

Objective:

- Understand the flame stabilization
- Identify the modes of combustion
- Quantify the role of autoignition

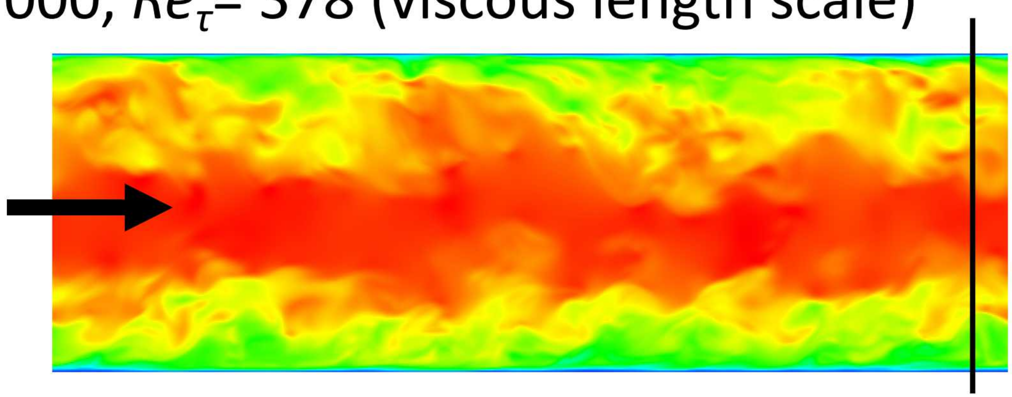
Simulation details



1.25 billion grid points
20 million CPU hours
$Re_b = 13000$

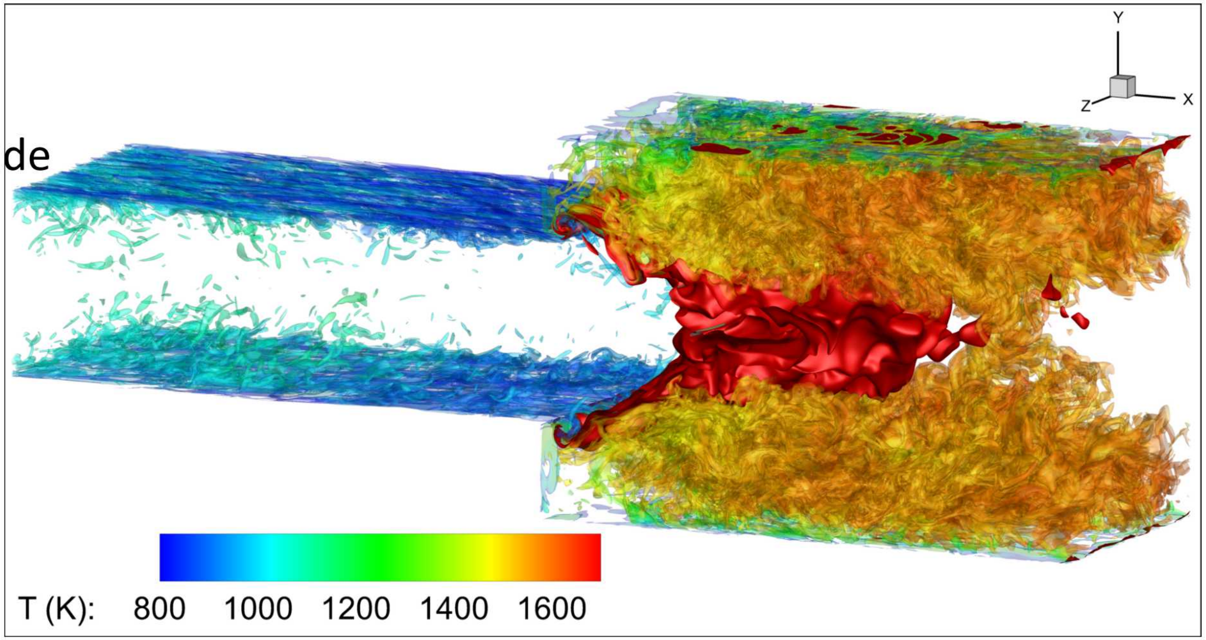
- **Chemical mechanism:** 9 species hydrogen-air (Li et al., 2004)
- **Inflow composition:** premixed $H_2 + O_2 + N_2 + H_2O$ ($\phi = 0.35$)
- Ubulk = 200m/s, u' = 20m/s, T_{inlet} = 1100K, T_{wall} = 750K
- **Inflow profile:** feed from DNS of a fully developed channel flow,

$Re_b \sim 13,000$, $Re_\tau = 378$ (viscous length scale)



Enstrophy conditioned on temperature, and heat release rate (red)

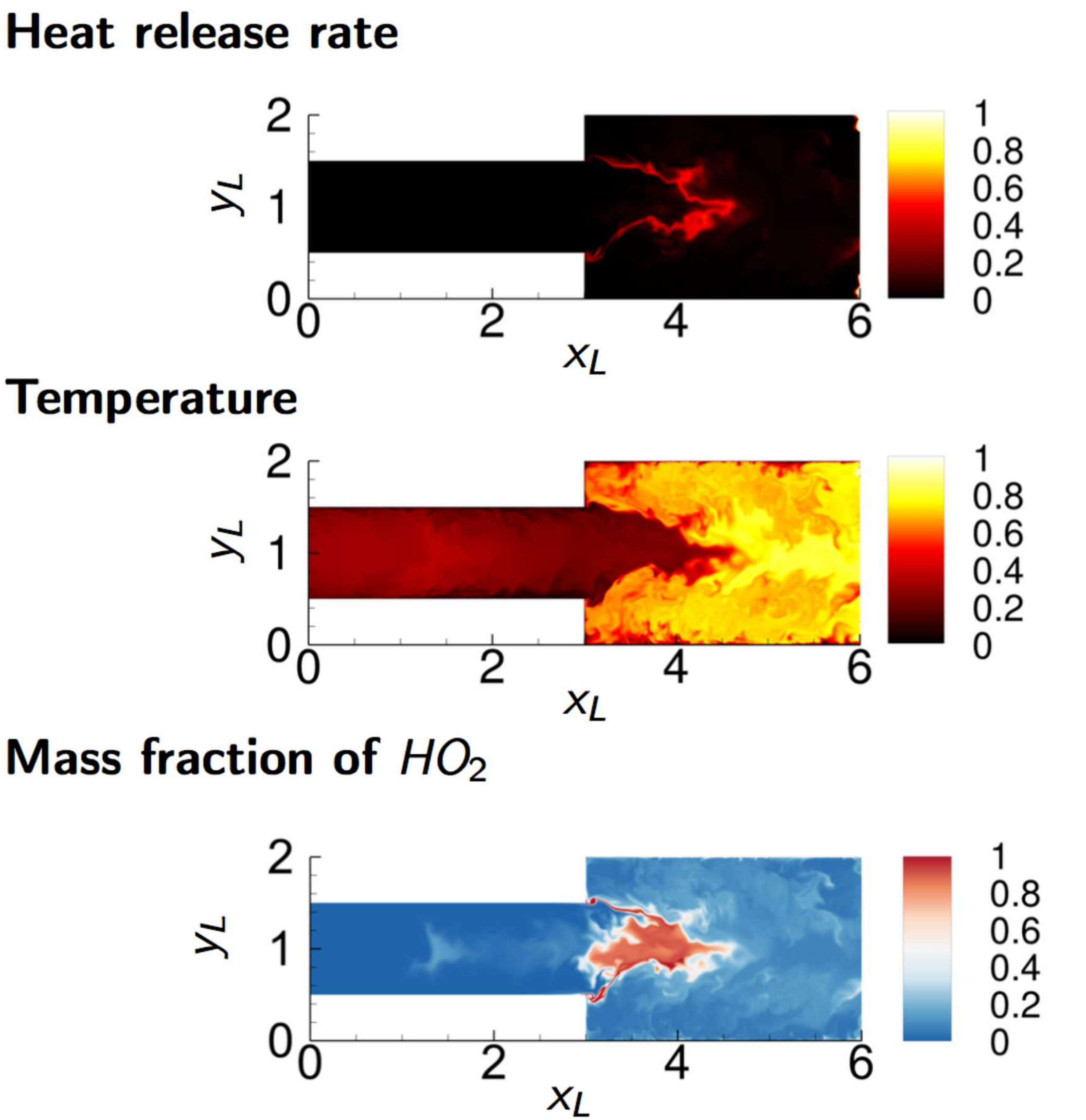
Iso-surfaces of vorticity magnitude colored by temperature



Two combustion configurations are observed:

- Design state: mainly auto-ignition in the combustion chamber
- Intermittent auto-ignition state: ignition in mixing section

Design combustion state



Combustion modes:

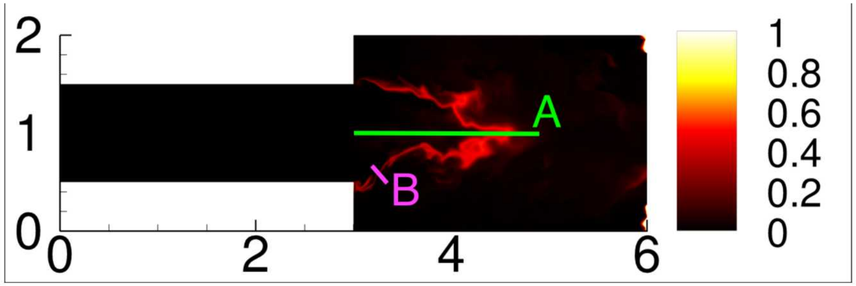
- Autoignition along center-line
- Flame propagation near corners
- HO2: indicative of chain branching

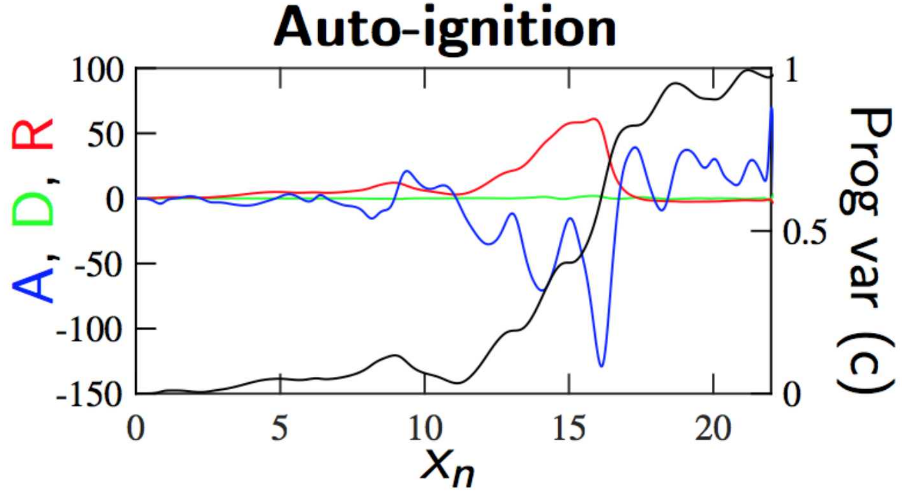
Combustion mode: OH budget analysis

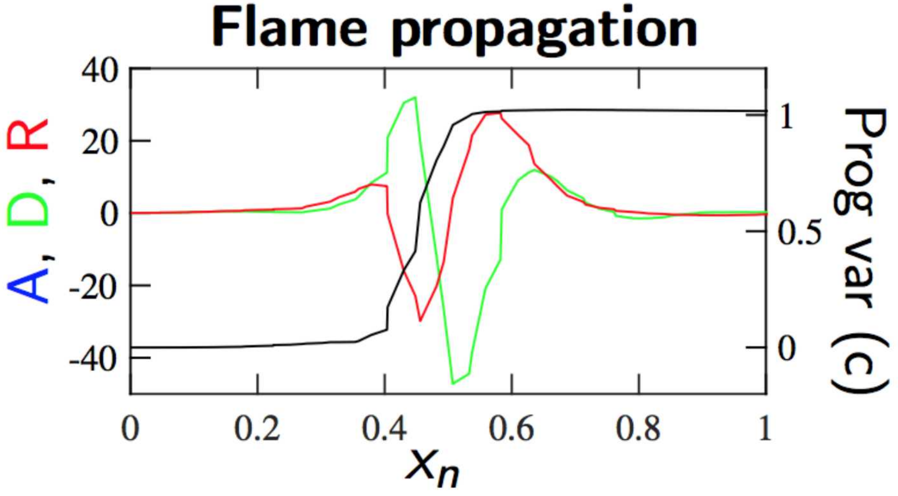
$$\frac{\partial(\rho Y_{OH})}{\partial t} = -\nabla_\beta \cdot (\rho Y_{OH} \mathbf{u}_\beta) - \nabla_\beta \cdot (\rho Y_{OH} \mathbf{V}_{\beta,OH}) + W_{OH}\dot{\omega}_{OH}$$

Advection Diffusion Reaction

- Auto-ignition: balance between advection and reaction
- Flame propagation: balance between diffusion and reaction

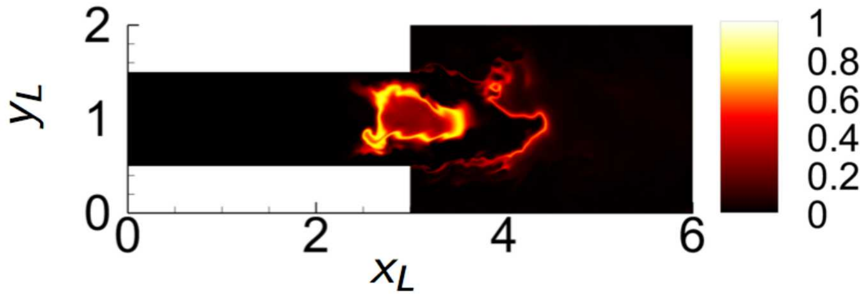




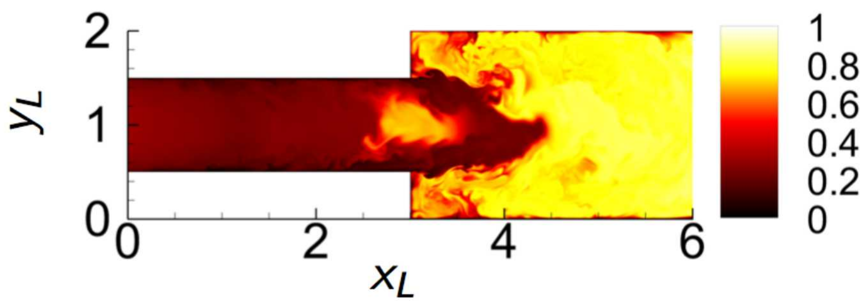


Intermittent auto-ignition state

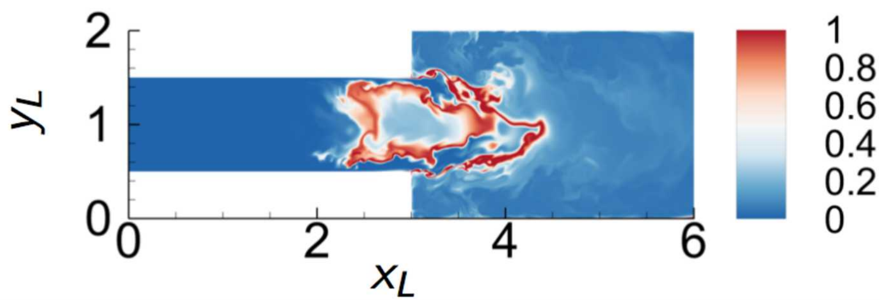
Heat release rate



Temperature



Mass fraction of HO_2



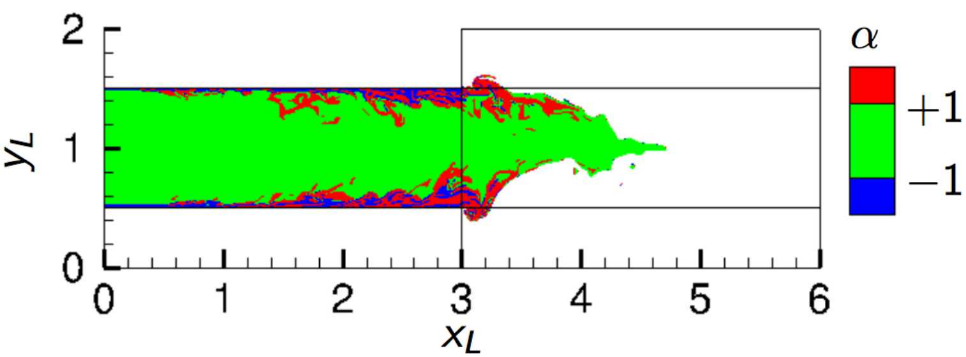
- Early auto-ignition in the mixing section
- Ignition kernel advects downstream
- Occurs intermittently

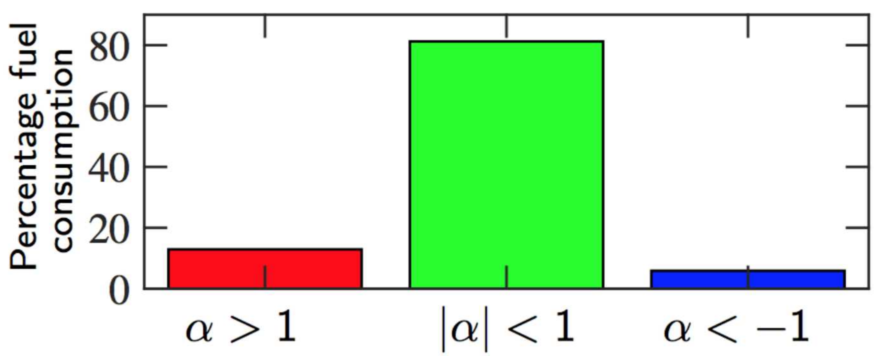
Chemical Explosive Mode Analysis

• $\alpha = \phi_s / \phi_\omega$: ratio of the projected non-chemical source term and the projected chemical source term (C. Xu et al., PROCI 2018)

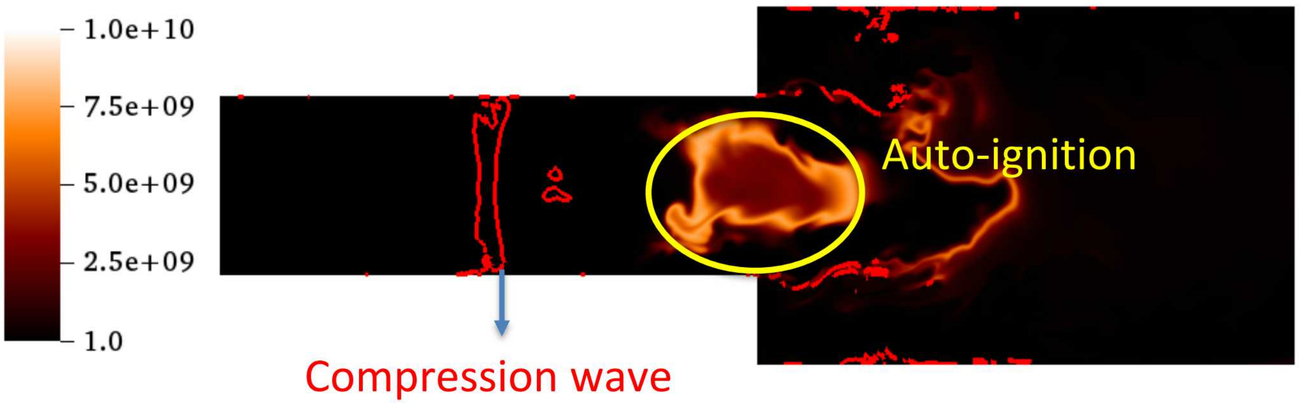
Three mode are identified:

• Assisted-ignition ($\alpha > 1$): diffusion significantly promotes reaction
• Auto-ignition ($-1 < \alpha < 1$): chemistry plays a dominant role
• Extinction zone ($\alpha < -1$): diffusion dominates chemistry and suppresses ignition

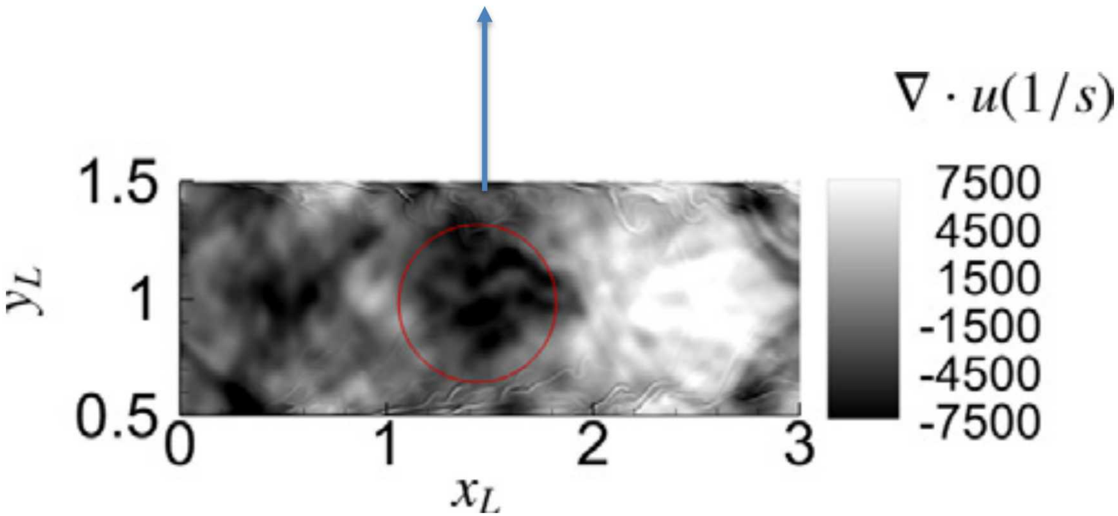




Intermittent auto-ignition state



Contours of heat release



Contours of instantaneous dilatation

- Local rise in pressure due to intermittent constructive interference pattern
- Increases local temperature by 20-30 K
- High reactivity of hydrogen
- Decrease in ignition delay time (30%)

Conclusions

- Performed DNS of a reheat burner at scaled conditions
- Two states of hydrogen/air combustion have been observed:
  - design state: flame propagation and auto-ignition in the combustor
  - intermittent auto-ignition in mixing section
- Premature auto-ignition arises due to pressure (and following temperature) rise in mixing section
- Quantified the contribution of different modes towards heat release using chemically explosive mode analysis (CEMA)
- Future work:
  - characterize the unstable flame behavior and the conditions leading to it
  - find the inlet conditions for statistically stationary reheat flame
  - perform 2D and 3D simulations with varying fuel composition and its stratification

Parallel Programming 101 - Productivity

Functionally correct application code

Mapping to target machine

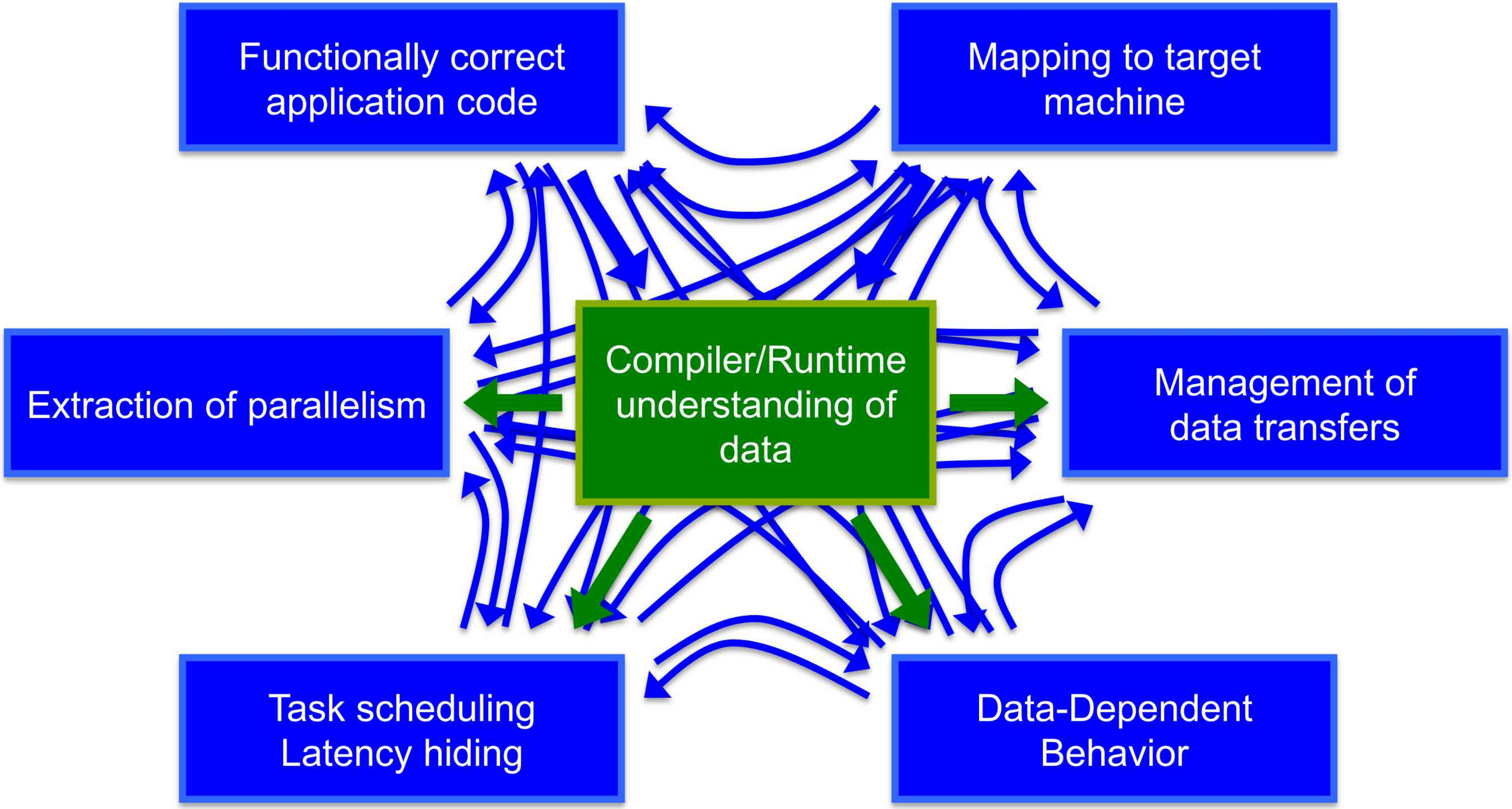
Extraction of para

anagement of
ata transfers

Task scheduling
Latency hiding

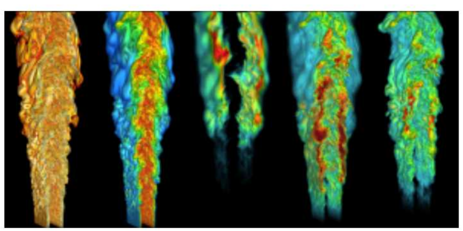
Data-Dependent Behavior

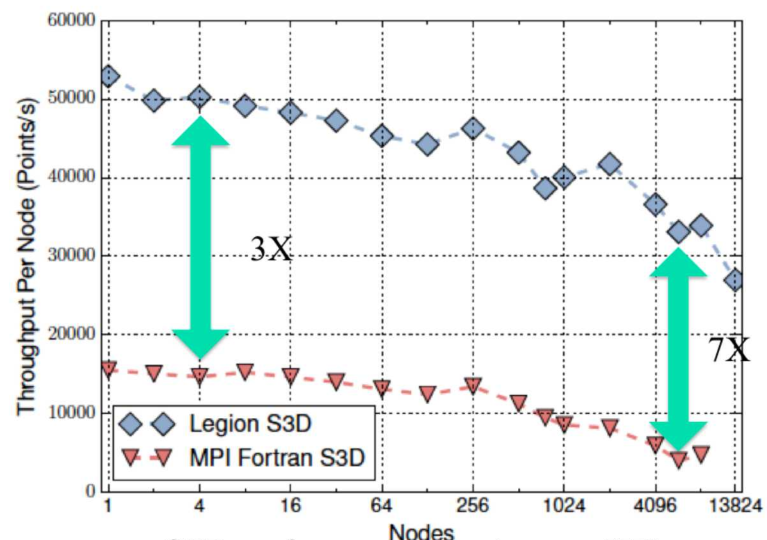
Parallel Programming 101



Legion Programming System applied to S3D

- A data-centric parallel programming system
- A programming model for heterogeneous, distributed machines
  - Automates many aspects of achieving high performance, such as extracting task- and data-level parallelism
  - Automates details of scheduling tasks and data movement (*performance optimization*)
  - Separates the specification of tasks and data from the mapping onto a machine (*performance portability*)
- Legion application example: S3D
  - Production combustion simulation
  - Written in ~200K lines of Fortran
  - Direct numerical simulation using explicit methods



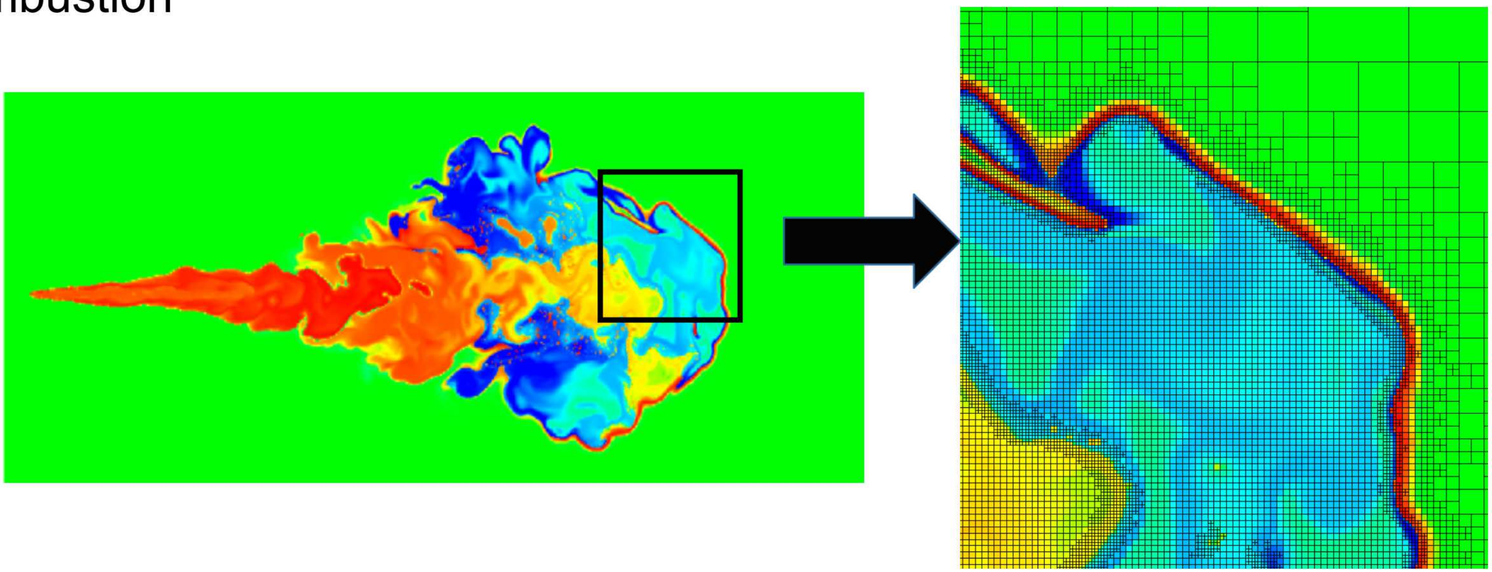


S3D performance Legion vs. MPI

S. Treichler et al., "S3D-Legion: An Exascale Software for Direct Numerical Simulation (DNS) of Turbulent Combustion with Complex Multicomponent Chemistry," CRC Book on Exascale Scientific Applications: Programming Approaches for Scalability Performance and Portability, 2017.

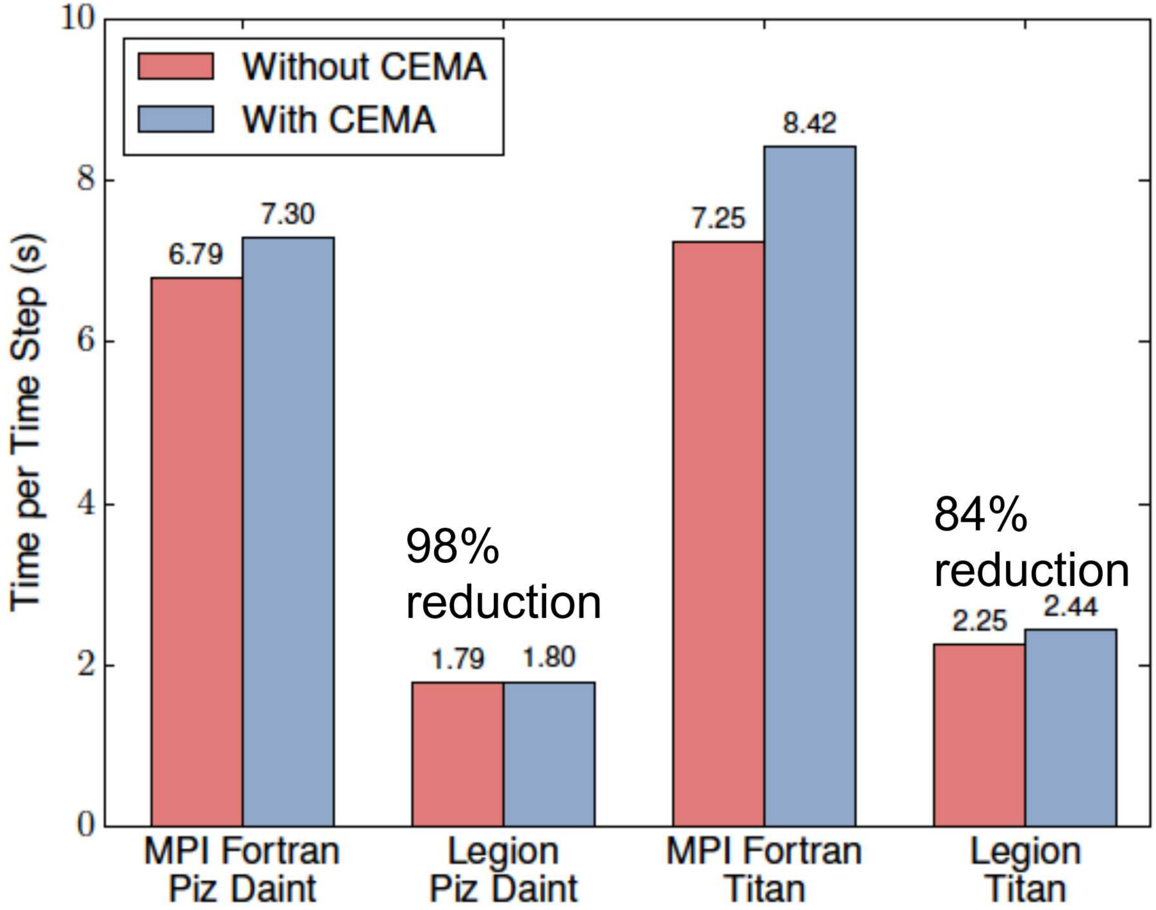
In-situ Data Analytics in Legion
Chemical Explosive Mode Analytics (CEMA)

- CEMA: eigenvalue solve on the reaction rate Jacobian to determine the mode of combustion



- Run CEMA at each time step as a diagnostic to steer mesh refinement
- CEMA computation takes longer than a single explicit RK stage (6 stages/timestep)
- Dividing CEMA across RK stages and interleaving with other computation so as not to impact other critical operations would be hard to schedule manually
- Asynchronous task execution, schedule CEMA on CPU resources
- Interoperate Fortran CEMA with Legion code – took a day to implement

Execution Overhead of In-situ Analytics (CEMA) in S3D-Legion (Titan & Piz Daint)



Legion S3D Lessons Learned

- Legion
  - S3D shows potential of data-centric, task-based models
  - Enables new simulation capabilities (physics, and in situ analytics)
  - Code is easier to modify and maintain
    - Ports are just new mappings, easy to tune for performance
    - New functionality usually just means new tasks
    - Legion will figure out the dependences and scheduling
    - Productivity requires higher level abstraction layer for scientists to write in

- Co-Design and ECP
  - The Legion/S3D experience is a tribute to co-design
  - Computer and computational scientists worked closely
  - Major progress on important problems resulted

Exascale Targets: Science at Relevant Conditions

- **Hybrid DNS/LES (near DNS) with dynamic adaptive mesh refinement, multi-physics (sprays, soot, radiation at high pressure) in geometry**
- **Reactivity Stratified Compression Ignition IC Engines** - multi-stage, high pressure autoignition of a liquid hydrocarbon fuel blend
- **Natural Gas IC Engines – ignition and knock**
- **Scramjets** – cavity stabilized shear driven lean turbulent premixed flames, effect of products recirculation coupled with high Re, high Ka, compressible flames
- **Gas Turbines** – swirl stabilized spray combustion gas turbines with lean premixed combustion, flame stabilization, nitric oxide emissions, thermo-acoustics
- **Include in-situ analytics & visualization**