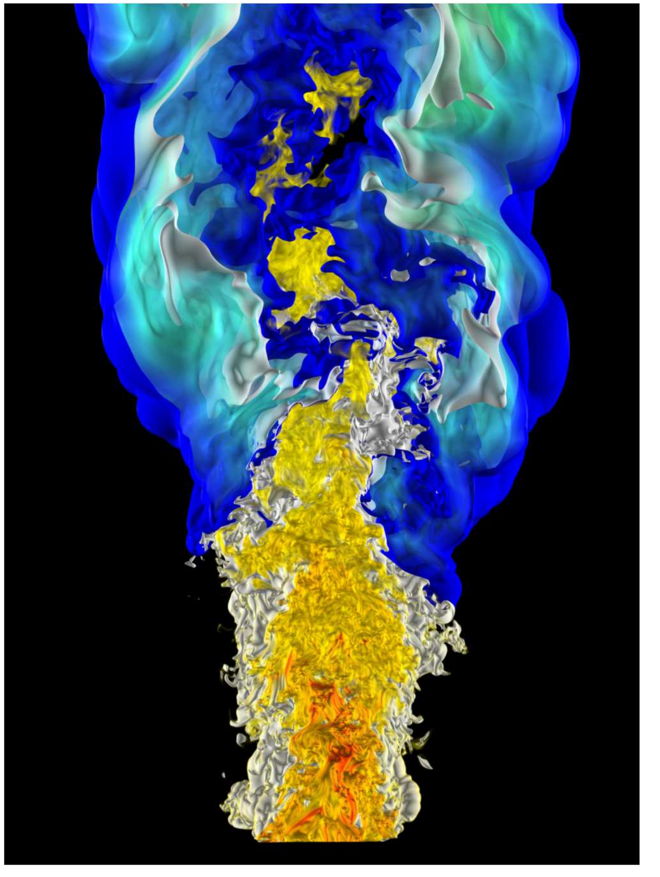
This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

DNS of Autoignition of Diesel Surrogate Fuel in a Turbulent Jet at High Pressure with S3D-Legion on Titan/Summit

SAND2019-5000C



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SIAM 17th International Conference on Numerical Combustion, Aachen, Germany
May 6-8, 2019

Office of Science
U.S. Department of Energy

Sandia National Laboratories

ECP Exascale Computing Project

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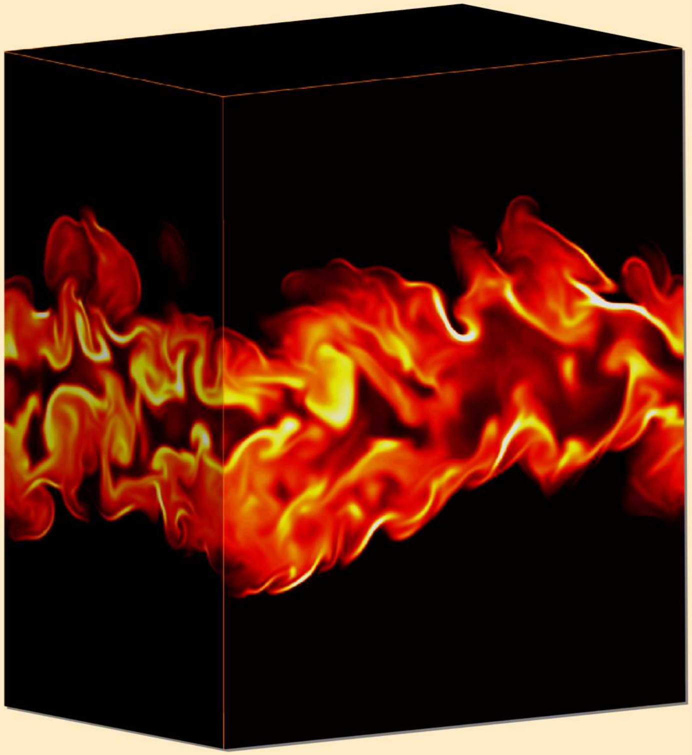
Direct Numerical Simulation – S3D

- 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

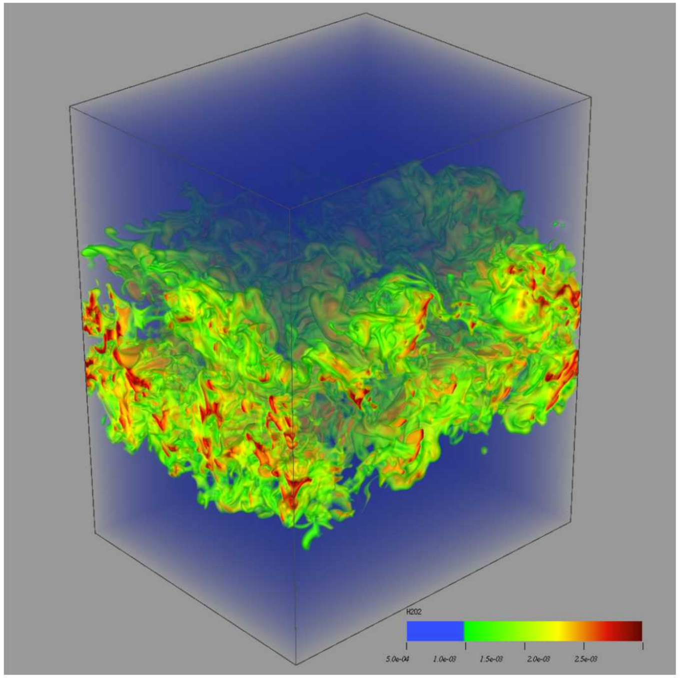
Chen *et al.*, *Comp. Sci. Disc.*, 2009

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

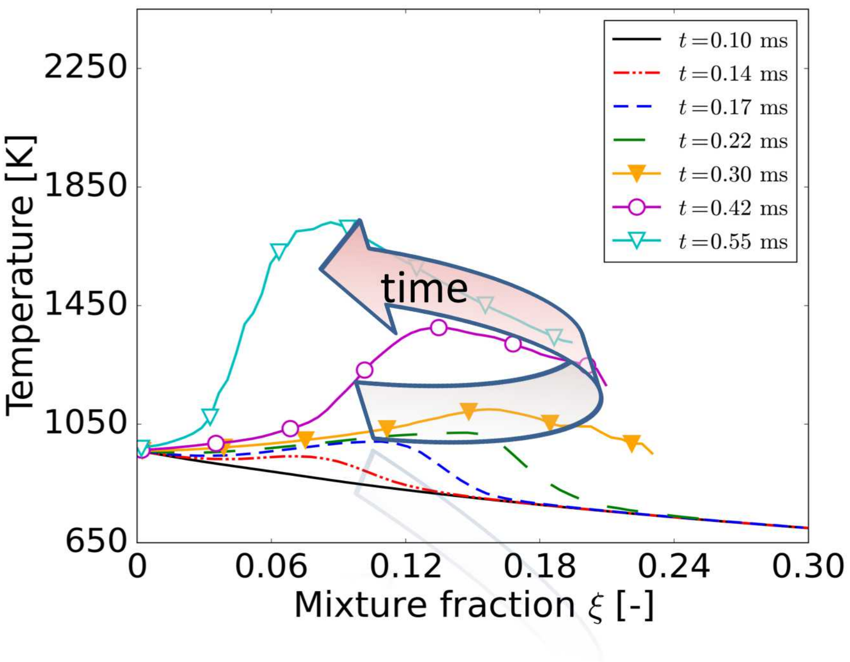


Ketohydroperoxide mass fraction

Borghesi et al. Combustion and Flame, 2018

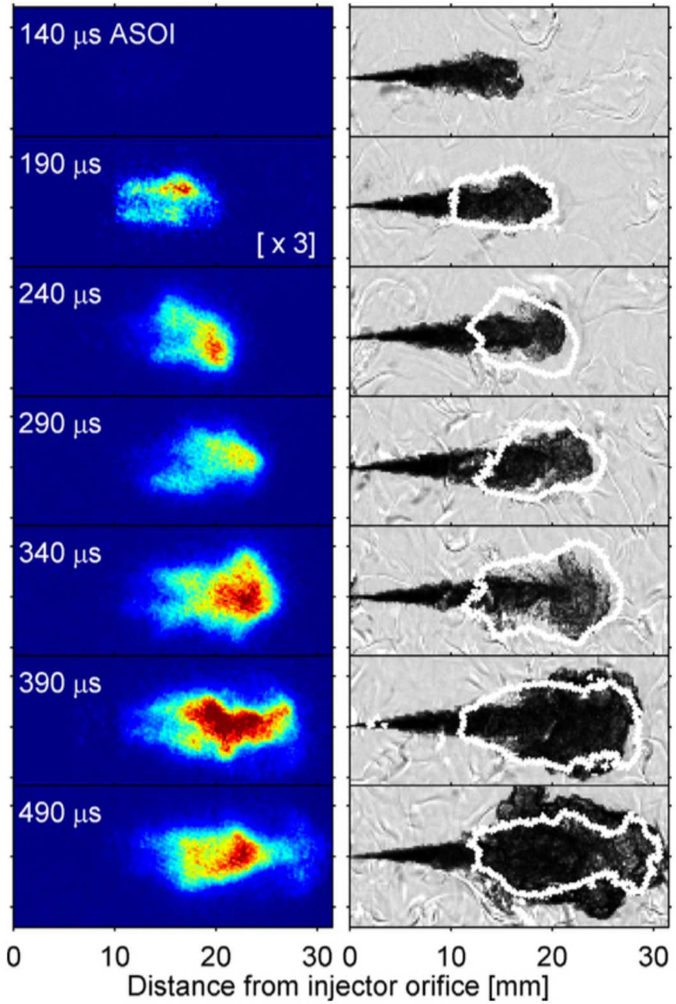
Background and Objective

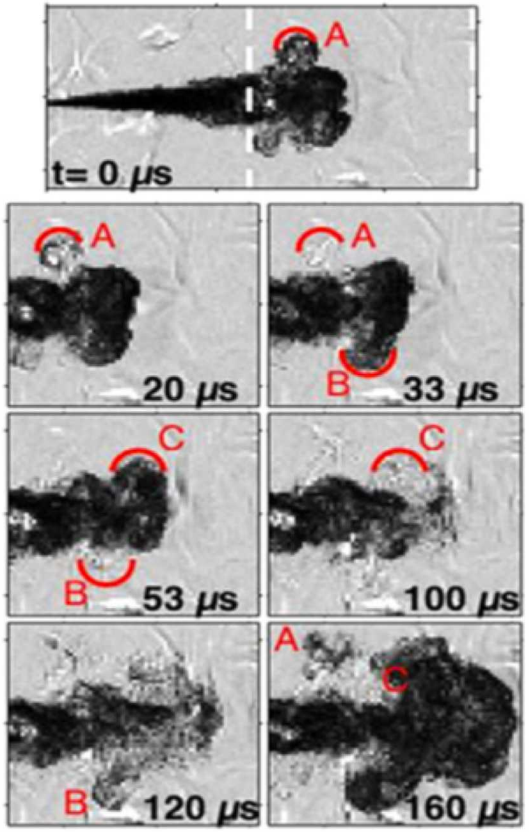
- Low-temperature combustion (LTC) aims at increasing fuel efficiency and reducing emissions
- Under LTC conditions, combustion occurs in a mixed mode and in multiple ignition stages
- Ignition is now very sensitive to the fuel chemistry, especially to the low temperature reactions branch

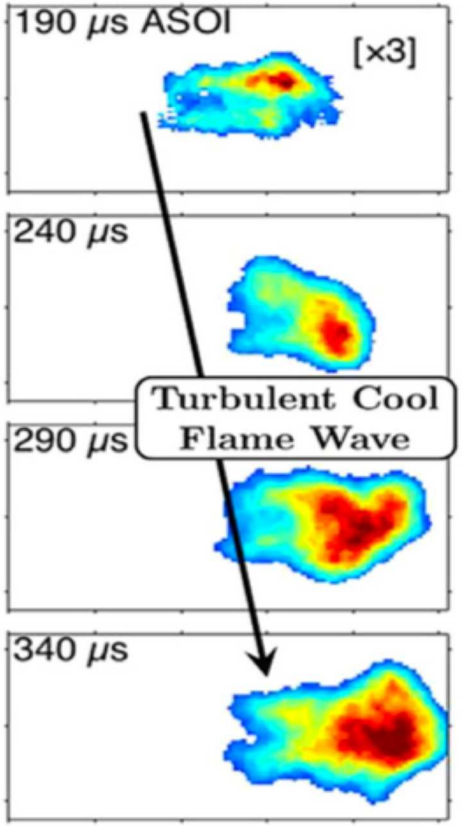


Question: How does transport and low-temperature chemistry affect ignition in low-temperature diesel combustion?

Low Temperature Diesel Combustion Experiments – Engine Combustion Network





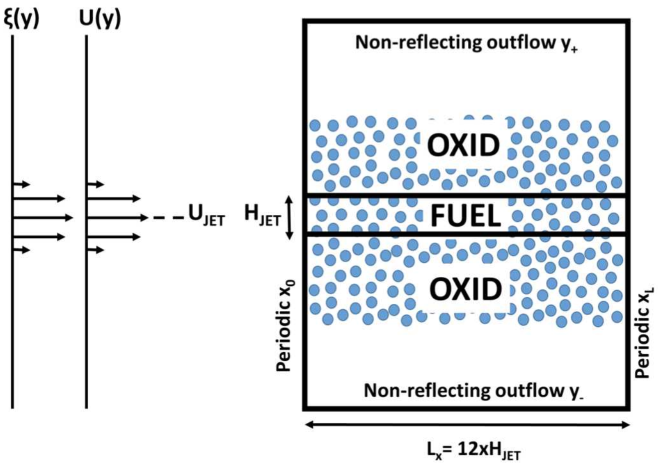


Skeen et al., PROCI 35 (2015) 3167-3174

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

DNS Configuration and Physical Parameters

- **Pressure:** 25 bar
- **Air stream:** 21% X_{O2}+79% 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



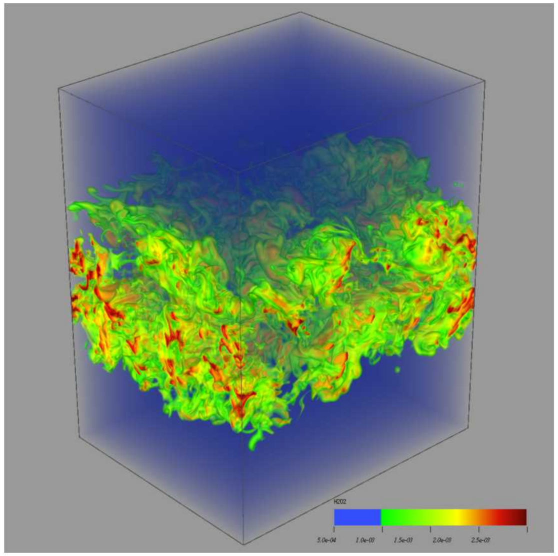
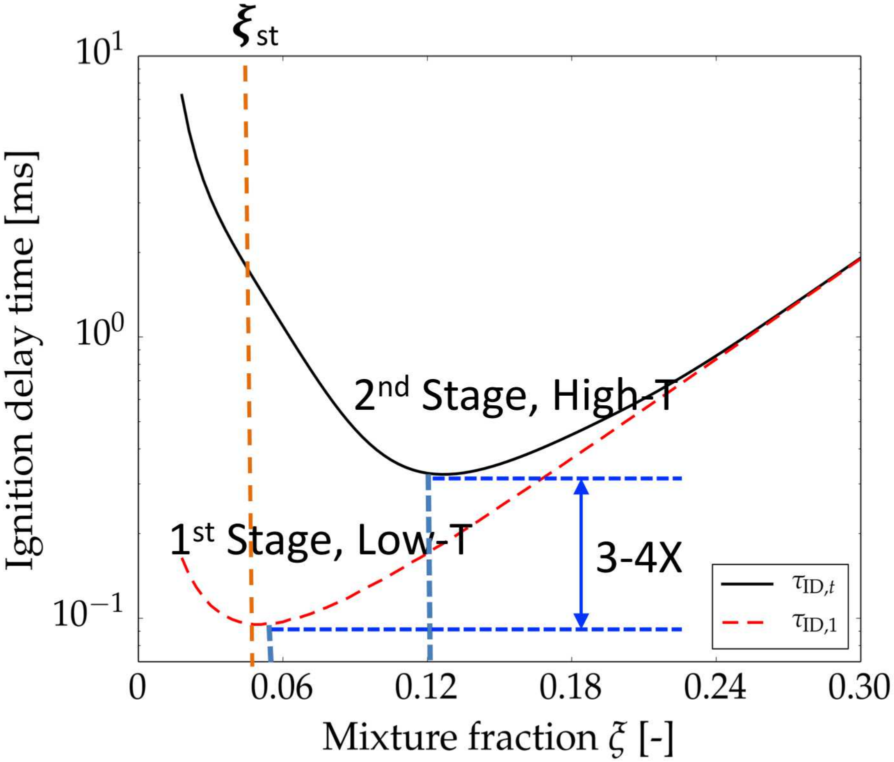
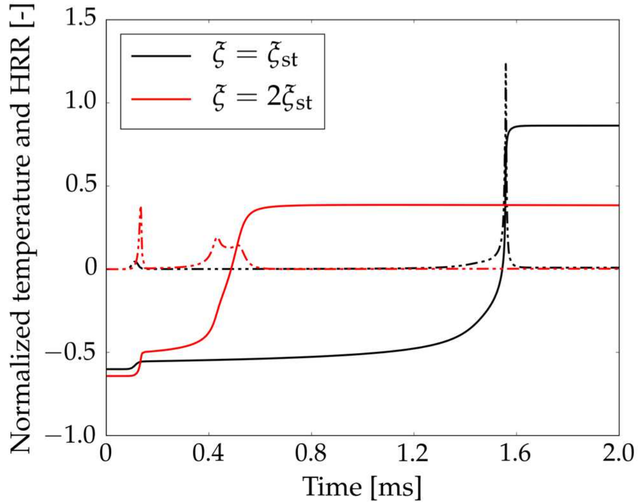
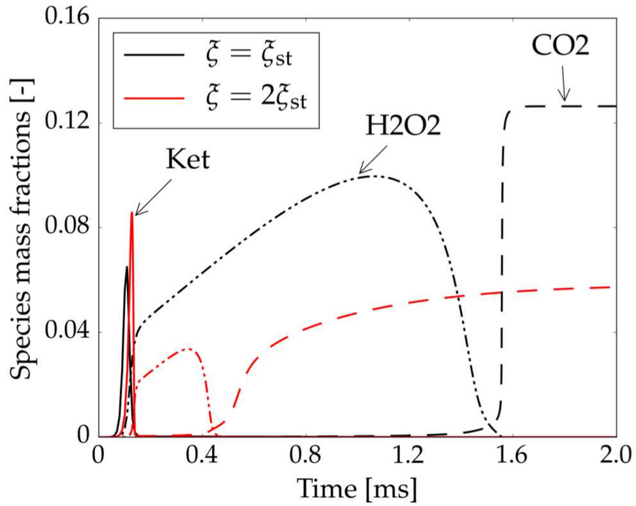


Figure: H_2O_2 mass fraction at t=0.17 ms after start of reactions

Homogeneous Multi-Stage Autoignition



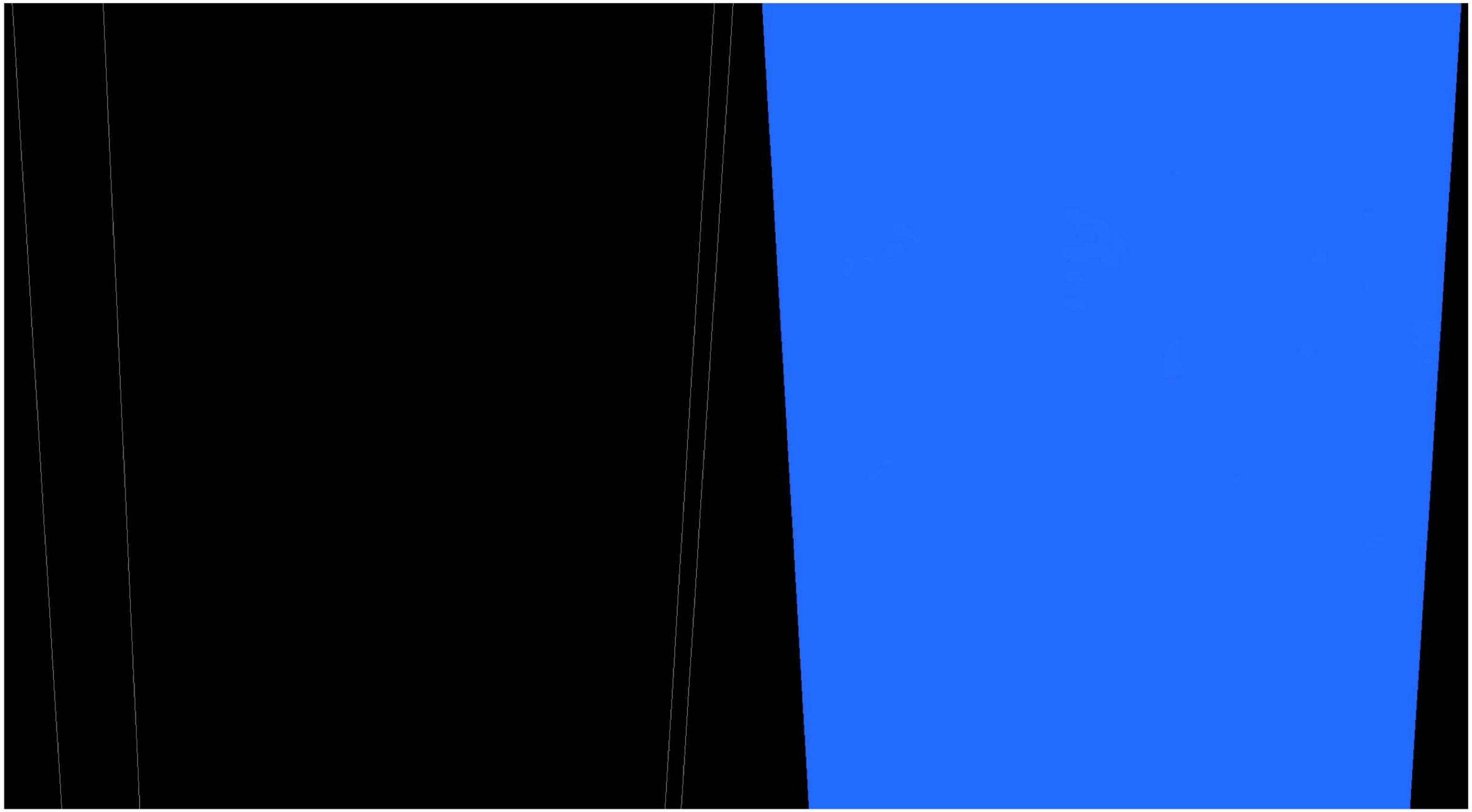




Homogeneous ignition delay time

Temporal evolution of selected reactive scalars

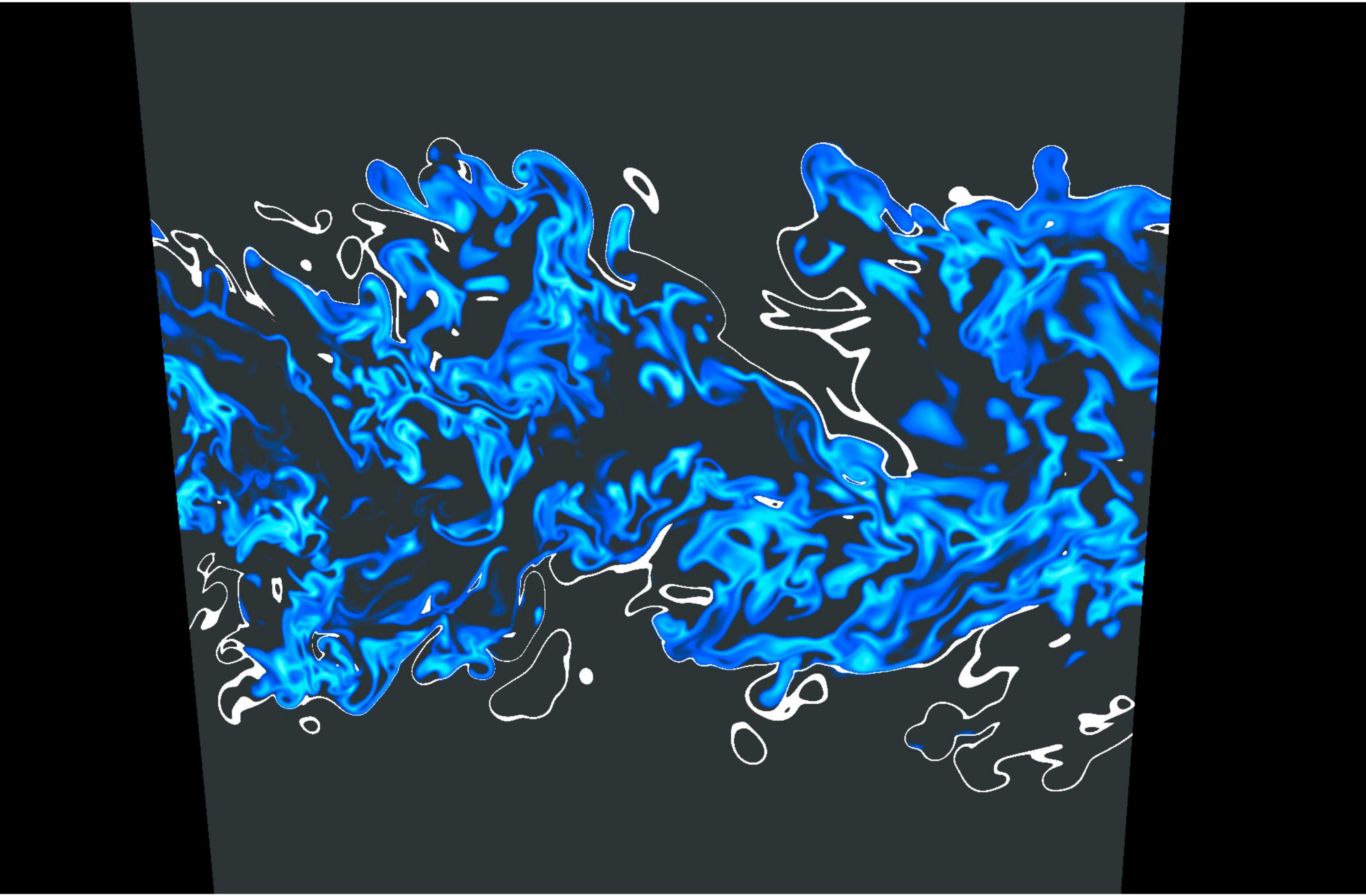
Dynamics of 2-Stage Ndodecane Ignition in a Jet at Diesel Conditions



Rendering by Chris Ye, Min Shih, Franz Sauer, and Kwan-Liu Ma

Ketohydroperoxide and *T,K* (>1150K) **H_2O_2 mass fraction**

Ketohydroperoxide during low-T ignition



Conditional means Ket, H_2O_2, and Temperature

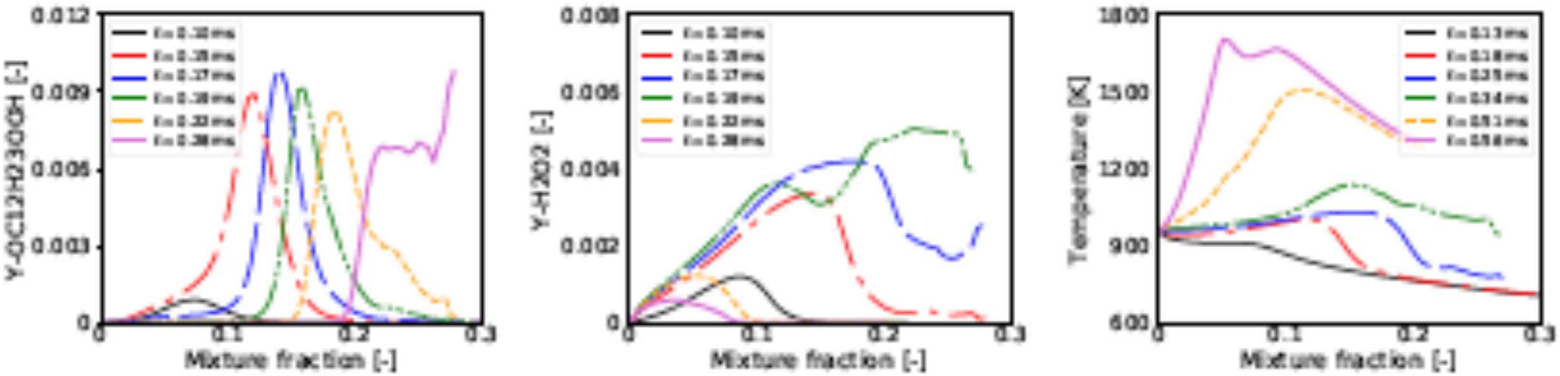
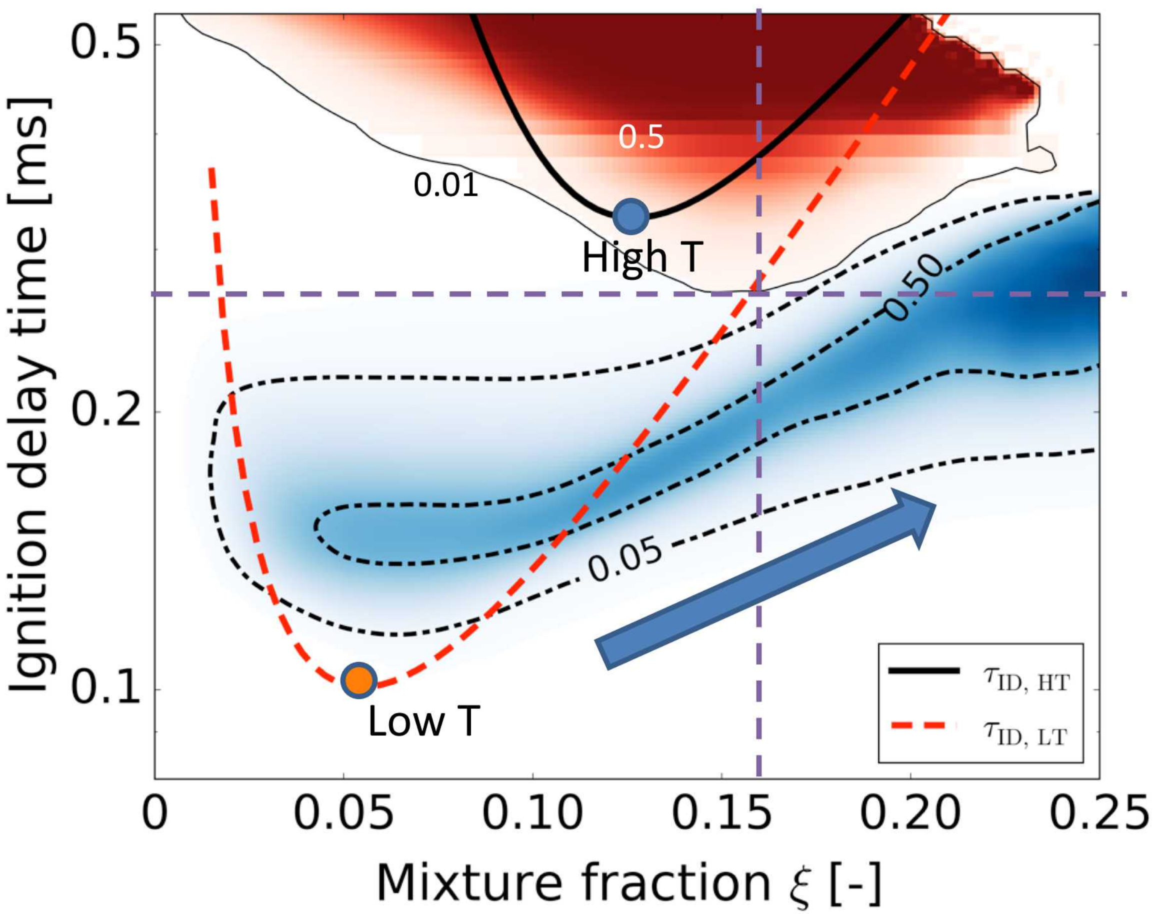


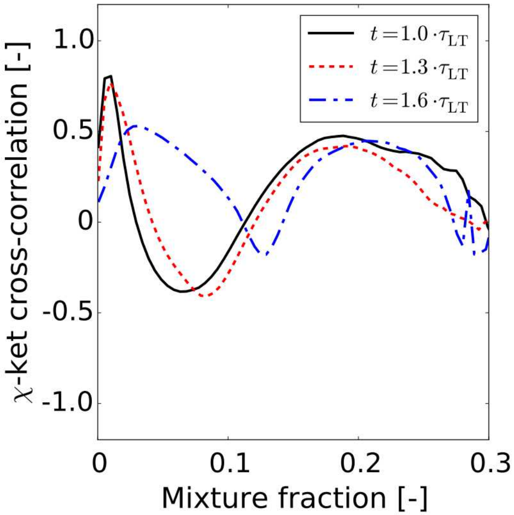
Fig. 2: Conditional mean ketohydroperoxide mass fraction (left image); hydrogen peroxide mass fraction (center image) and temperature (right image), conditioned on mixture fraction (fuel/air ratio) at selected times during low- and high-temperature autoignition of n-dodecane. The stoichiometric mixture fraction is at 0.046. A high-temperature flame is established by t = 0.56 ms. High-temperature ignition occurs first at a mixture fraction of 0.16 at 0.34 ms which is shorter than the corresponding homogeneous ignition delay.

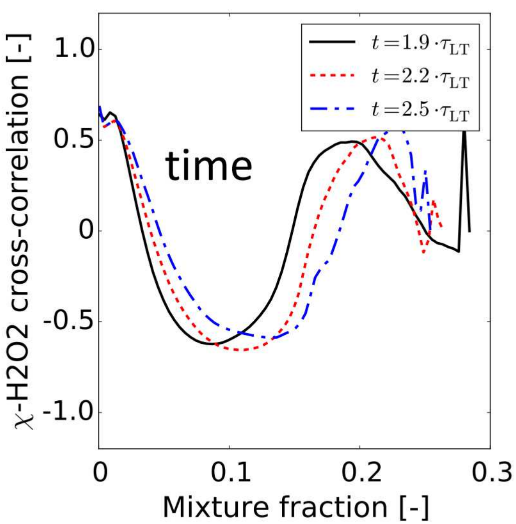
Turbulent versus homogeneous ignition

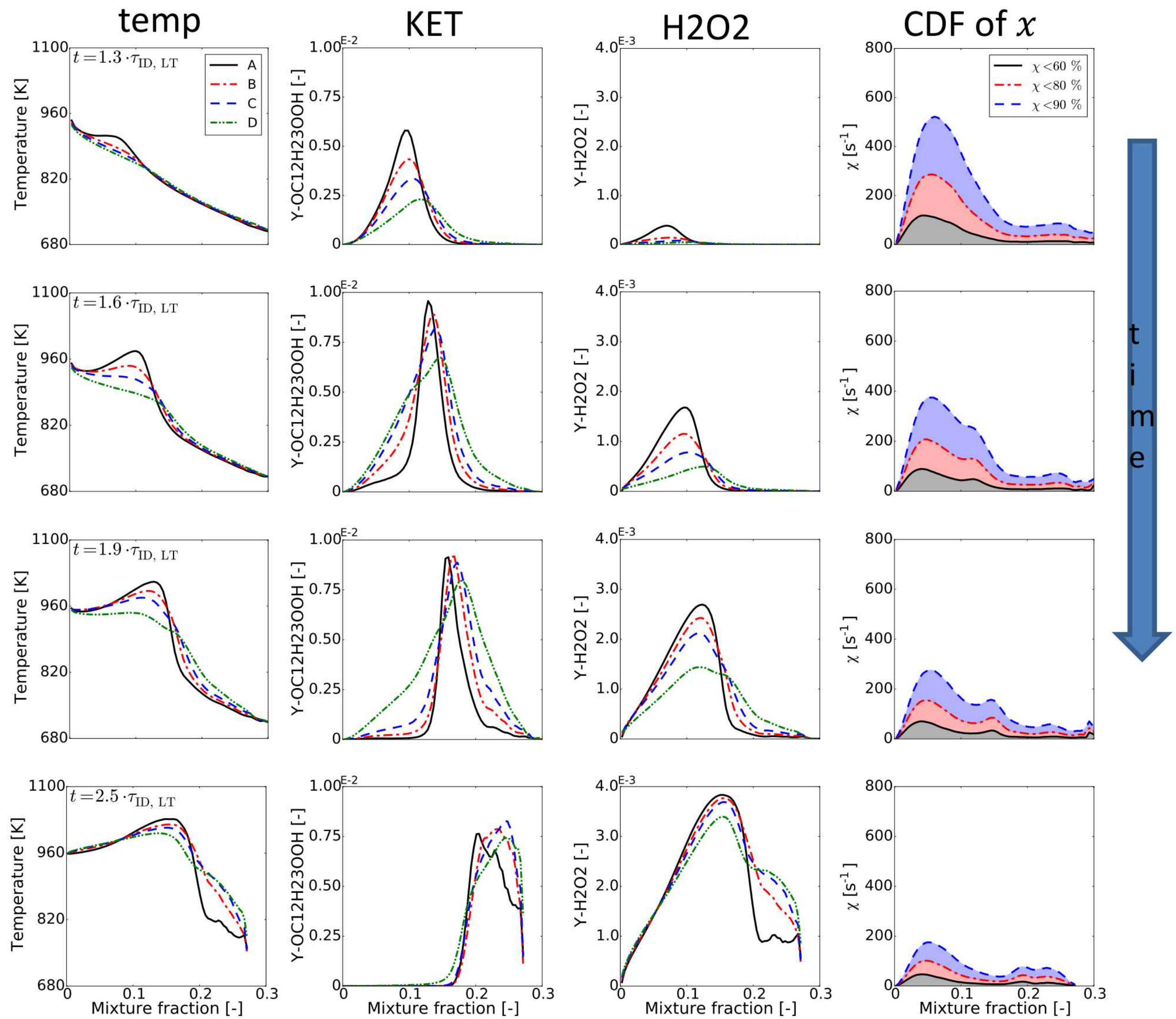


Low-T and high-T ignition in jet can be faster and than in a PSR !

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}.

Parallel Programming 101 - Productivity

Functionally correct application code

Mapping to target machine

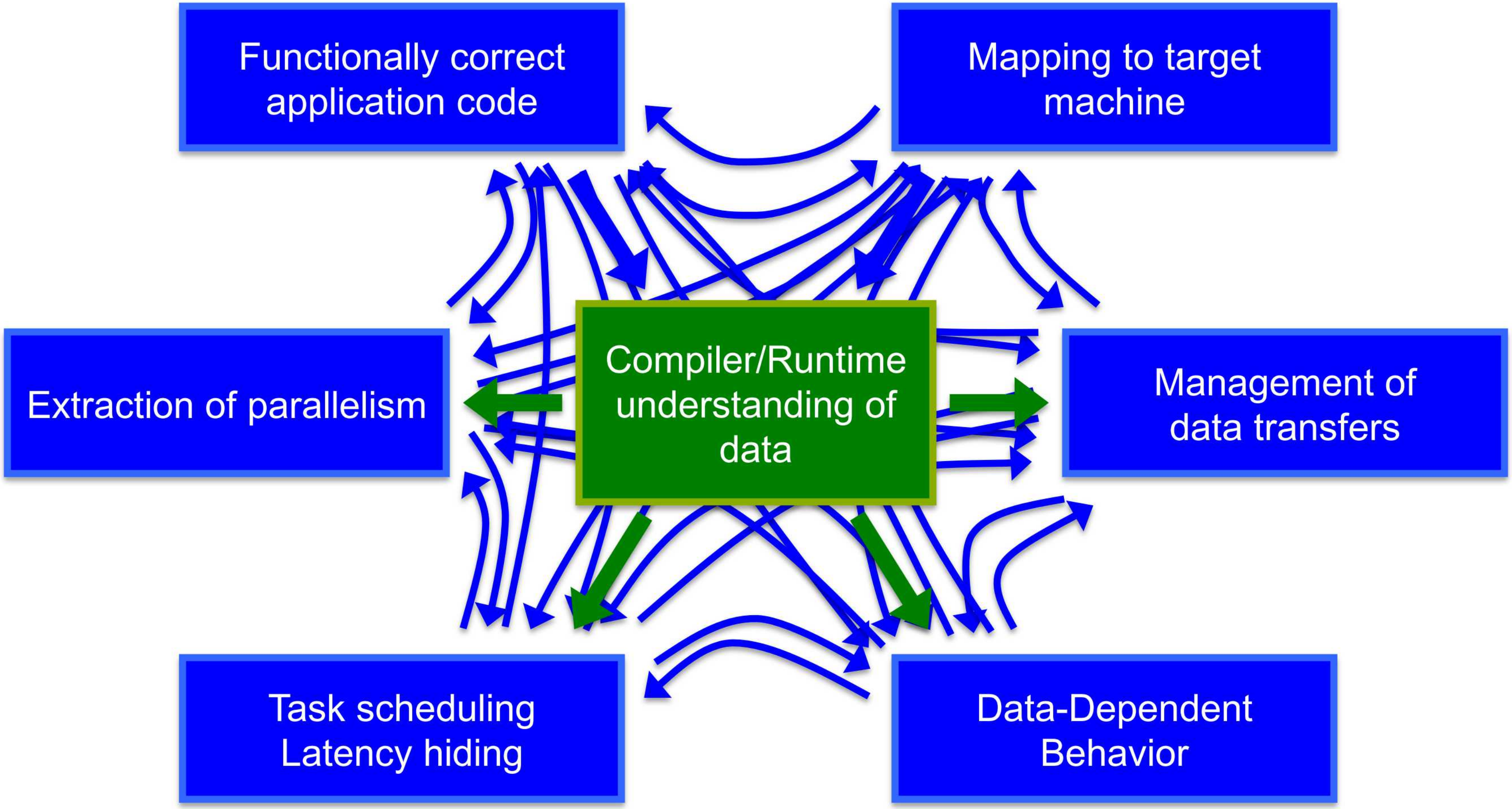
Extraction of para

anagement of ata transfers

Task scheduling
Latency hiding

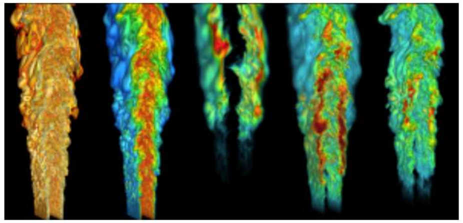
Data-Dependent Behavior

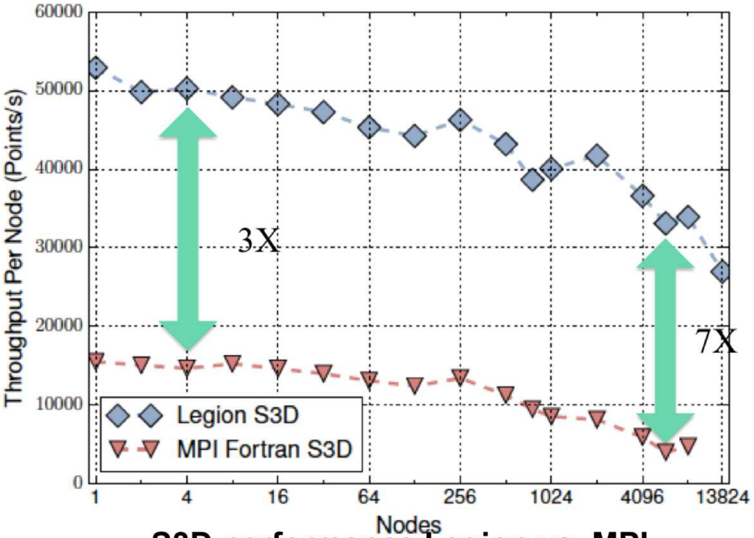
Parallel Programming 101



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.

ECP EXASCALE COMPUTING PROJECT

S3D-Legion Task Graph on a Summit node with n-dodecane chemistry (35 species)

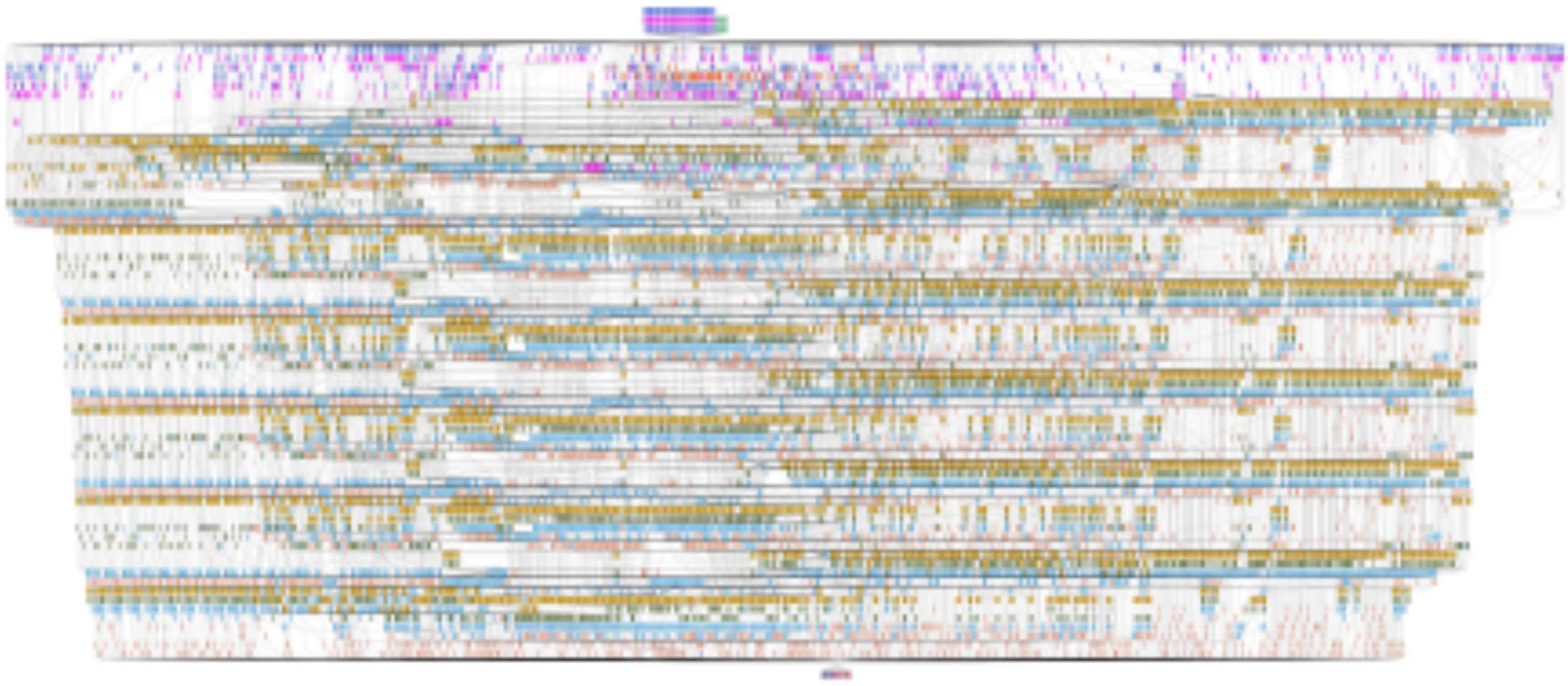


Fig. 3: The task graph for a single time step on one node of S3D-Legion simulating n-dodecane.

Weak and Strong Scaling Performance of S3D-Legion on Summit and PizDaint at ETH

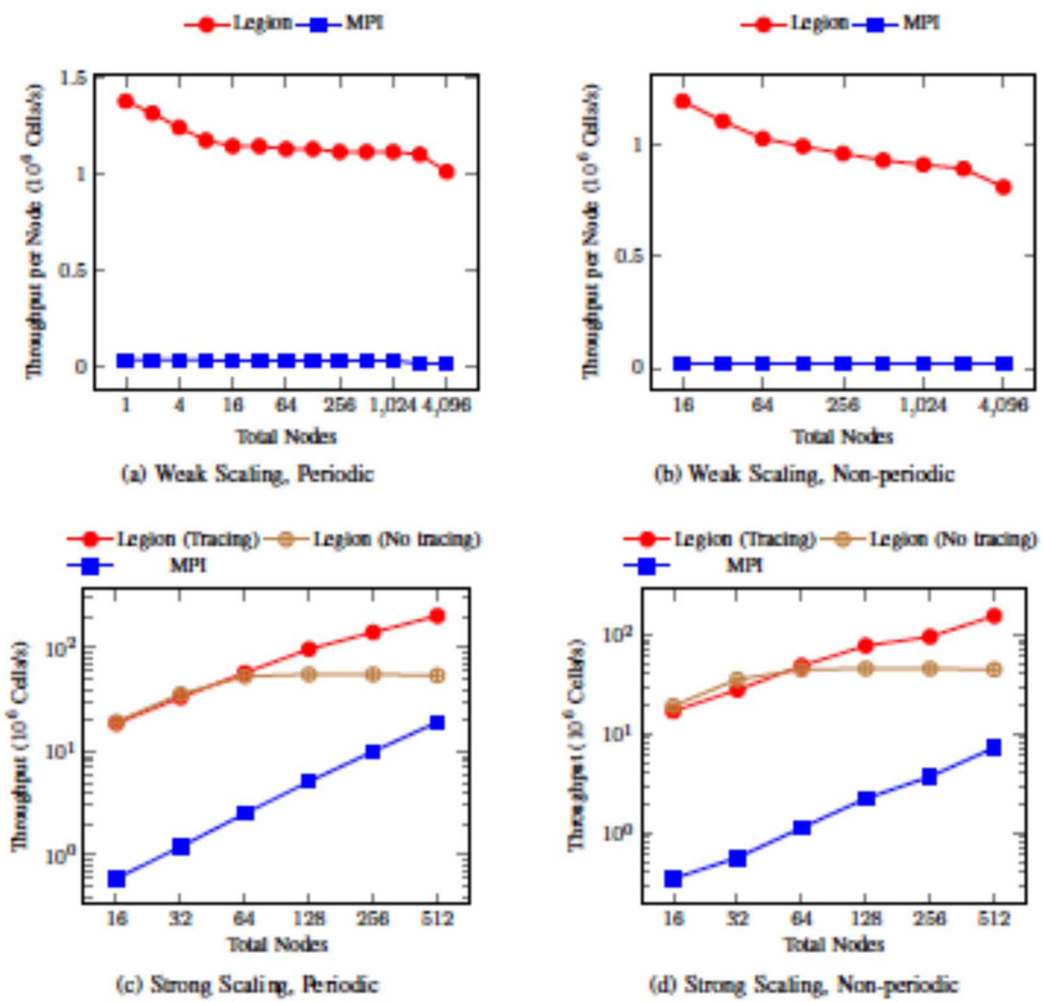
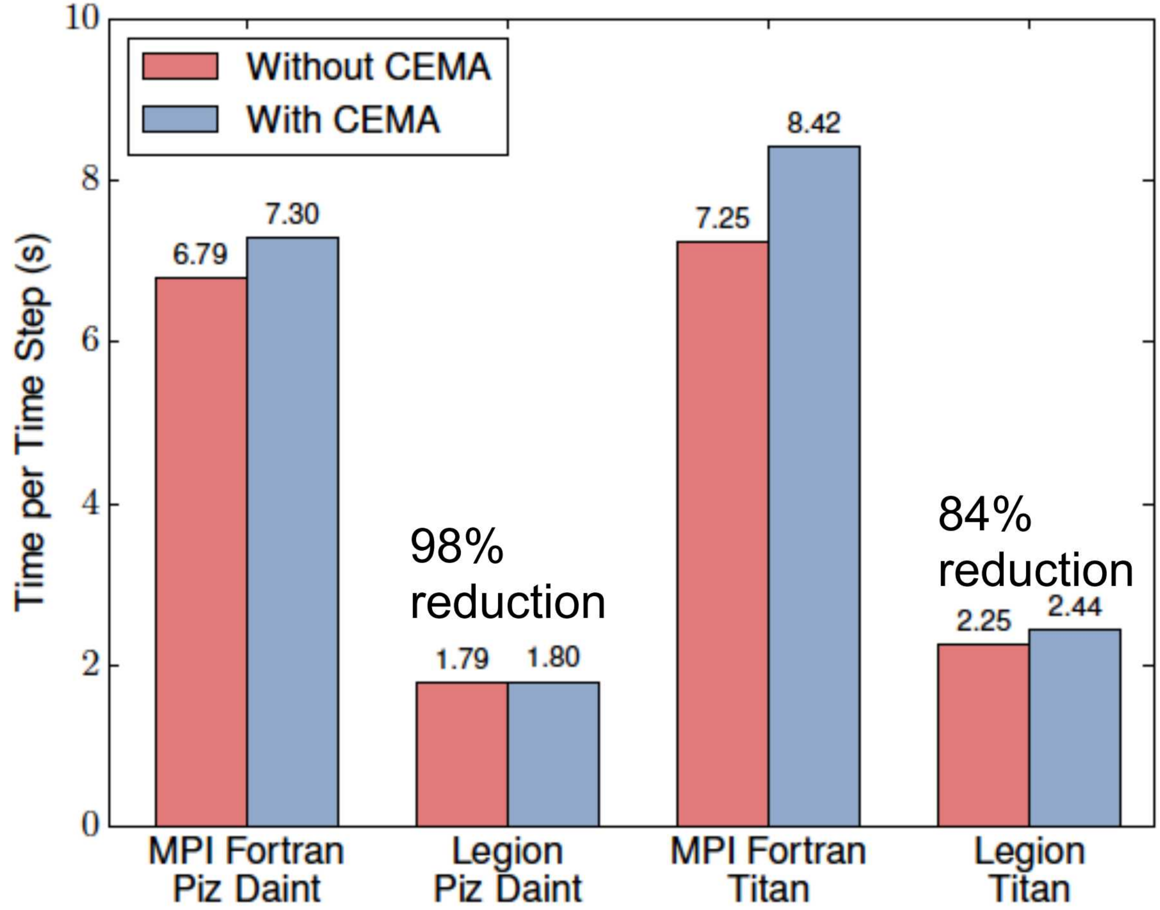


Fig. 4: Performance evaluation on Piz Daint

EXASCALE COMPUTING PROJECT

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