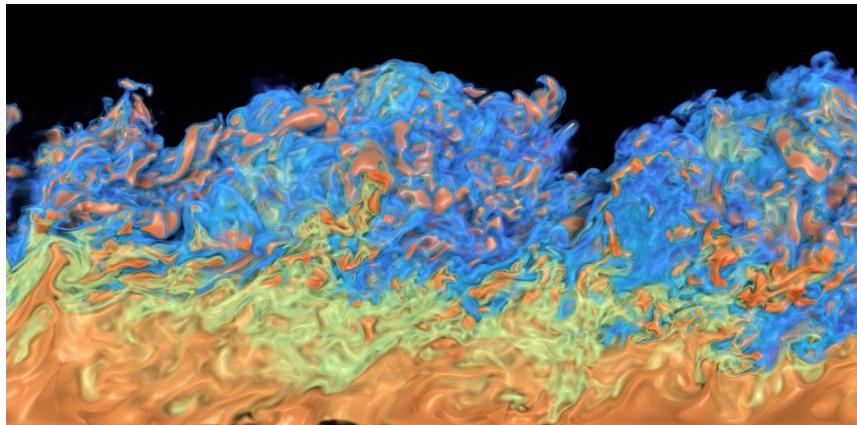


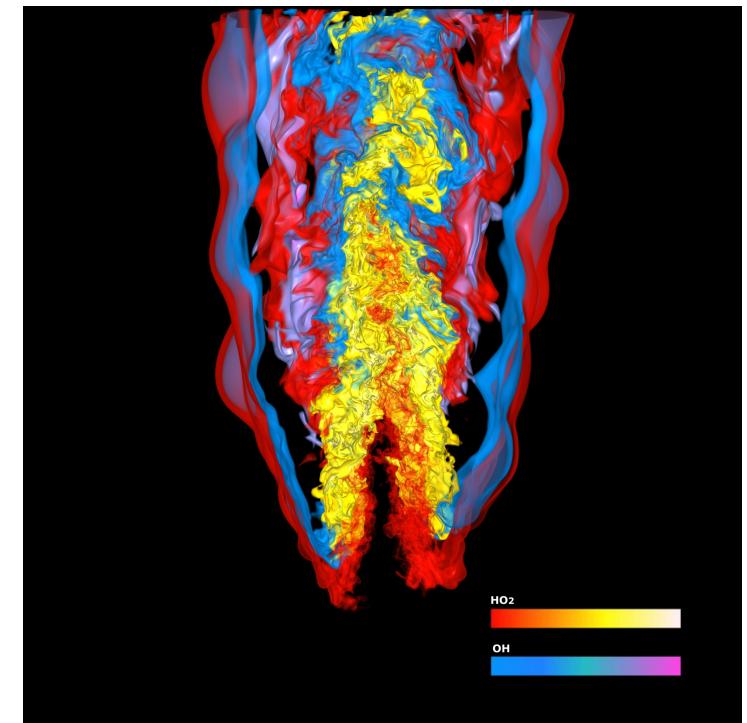
The Convergence of Exascale Computing, Data Science and Visualization Towards Zero Carbon Fuels for Power and Transportation



Temperature in a NH₃/H₂/N₂-Air Premixed Flame in a Shear Layer at 10 atm

Jacqueline Chen
Senior Scientist
Combustion Research Facility
Sandia National Laboratories
jhchen@sandia.gov

SC22 PAW-ATM Workshop
14 November, 2022
Dallas, Texas



HO₂ and OH in a lifted H₂/Air Jet Flame

Ammonia/hydrogen has the potential to be an alternative **zero-carbon** fuel for hard-to-electrify sectors: long-haul shipping, power generation and agriculture

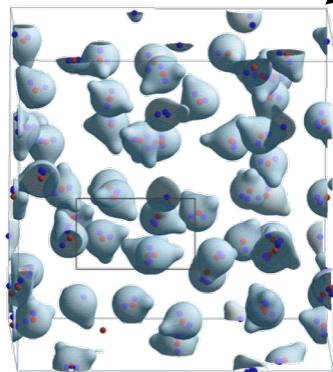


The convergence of exascale computing and data science

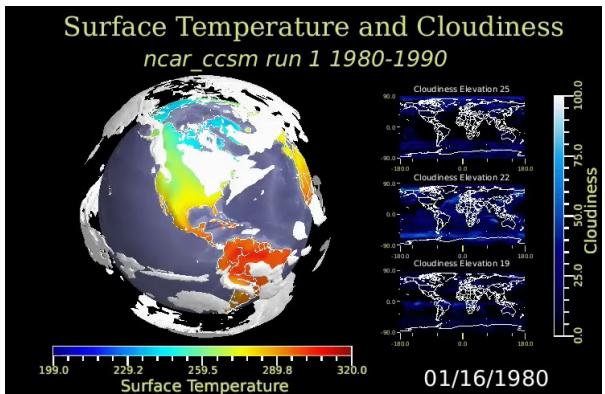
HPE/AMD
OLCF-5
(Frontier), 2
Exaflop 2022-
2023



Intel/HPE ALCF-3
(Aurora), 2 Exaflop,
2023-2024



Molecular Dynamics



Climate Modeling

Reduced Order
Surrogate
Models

In Situ Feature
Detection/Tracking,
Statistical
Aggregation and Viz

Combustion Modeling

$$\Phi(x, t) \approx U(x, t) \Sigma(t) Y(t)^T$$

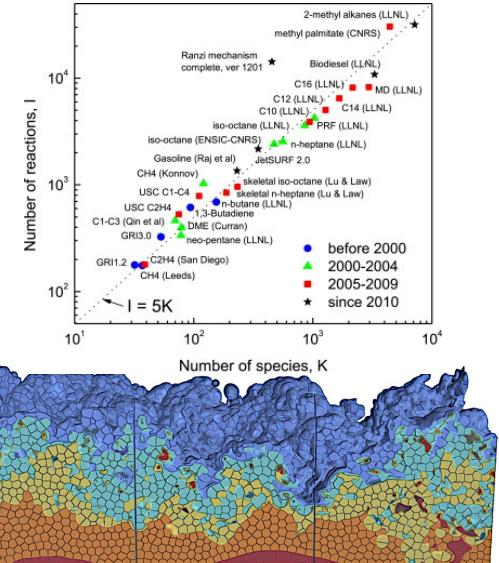
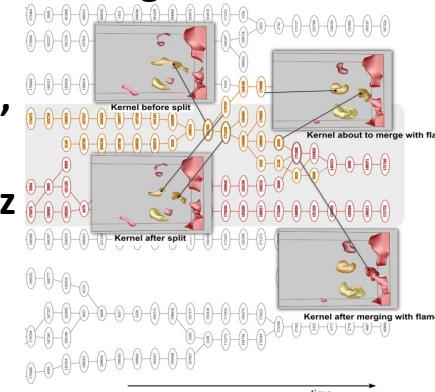
Reduced Order Surrogate Models

Matrix factorization diagram:

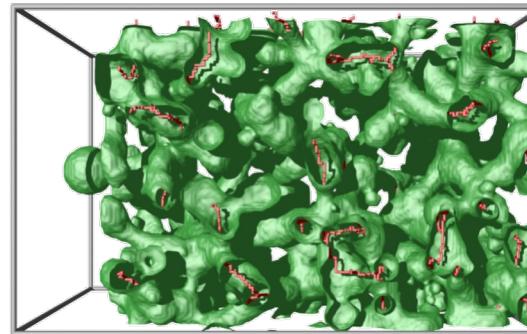
$$\Phi(x, t) \approx \begin{bmatrix} \cdots \\ U(x, t) \end{bmatrix} \begin{bmatrix} \cdots \\ \Sigma(t) \end{bmatrix} \begin{bmatrix} \cdots \\ Y(t)^T \end{bmatrix}$$

Dimensions: $\infty \times n_s$, $\infty \times r$, $r \times n_s$, $r \times n_s$

Merge Trees



Voronoi tessellation



Material Sciences

Direct Numerical Simulation of Turbulent Combustion: S3D

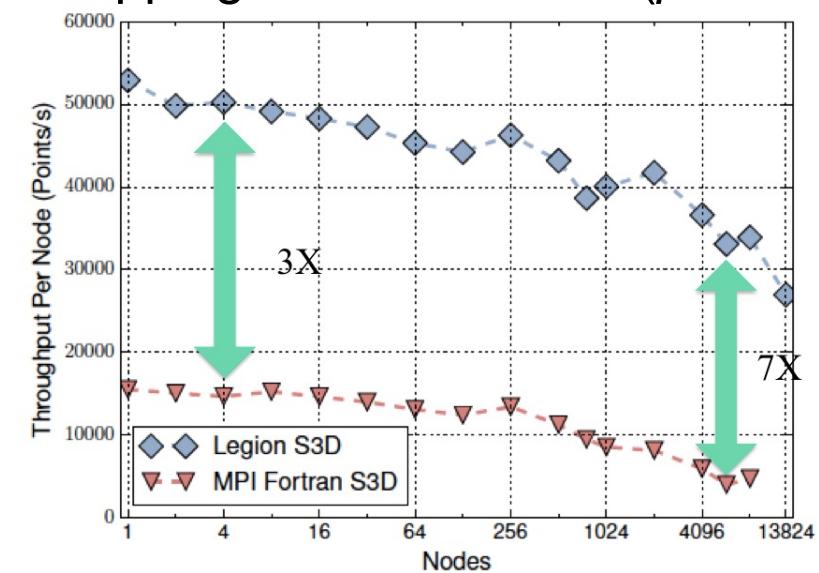
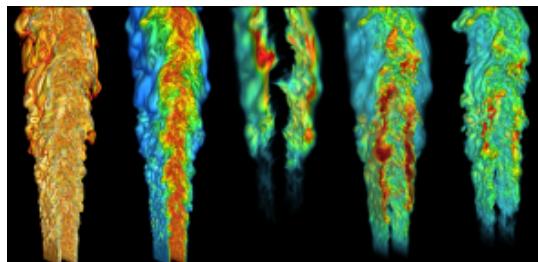
- Solves compressible reacting Navier-Stokes, total energy and species continuity equations
- High-order finite-difference methods
- Detailed reaction kinetics and molecular transport models
- Lagrangian particle tracking (tracers, spray, soot)
- Shock capturing
- Multi-temperature method (nonequilibrium)
- *In situ* analytics and visualization
- Geometry using immersed boundary method and multi-block approach
- Refactored for heterogeneous architectures using dynamic task based programming model (Legion/Regent)



DNS provides unique fundamental insight into the chemistry-turbulence interaction

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

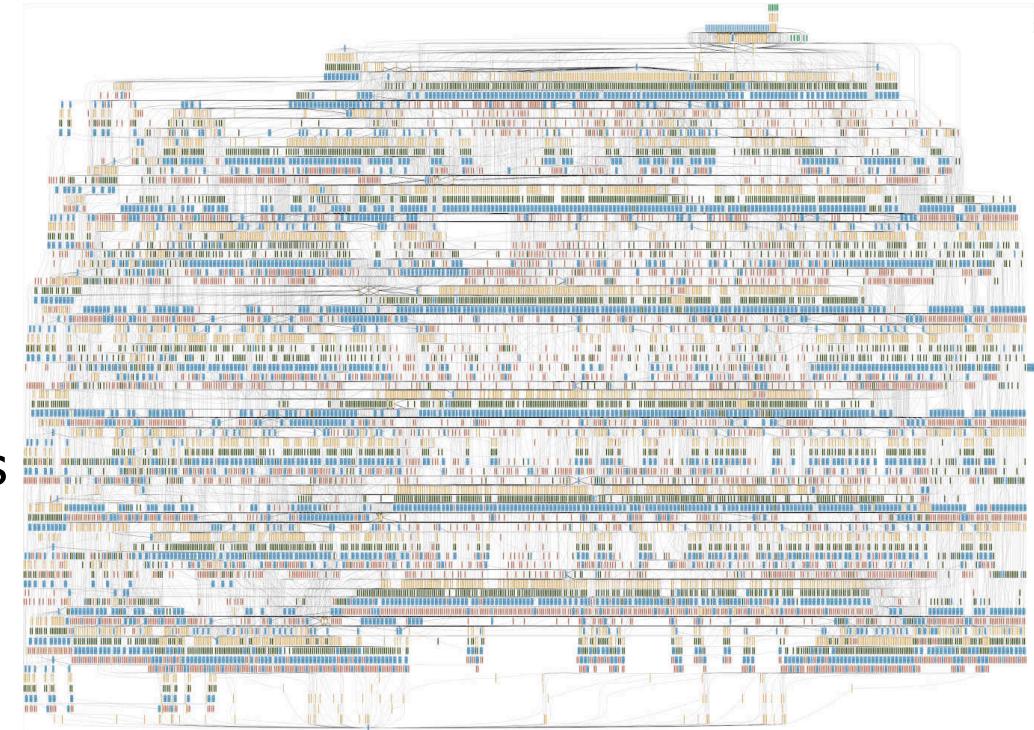


S3D performance Legion vs. MPI

Regent programming language applied to S3D Legion

- Regent is a programming language for task-based implicit parallelism
- Regent programs are composed of tasks (functions that perform computations on regions eligible for parallel execution) and logical regions (hierarchical collections of structured objects represented as cross-product of an index space and field space)
- Regent programs execute with sequential semantics with no explicit synchronization and a type system ensures program correctness on parallel/distributed machines
- Regent programs are transformed into efficient implementations for Legion
- Regent employs several novel compiler optimizations to minimize the dynamic overhead of the runtime system, especially at large node counts

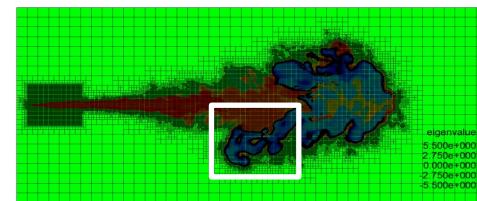
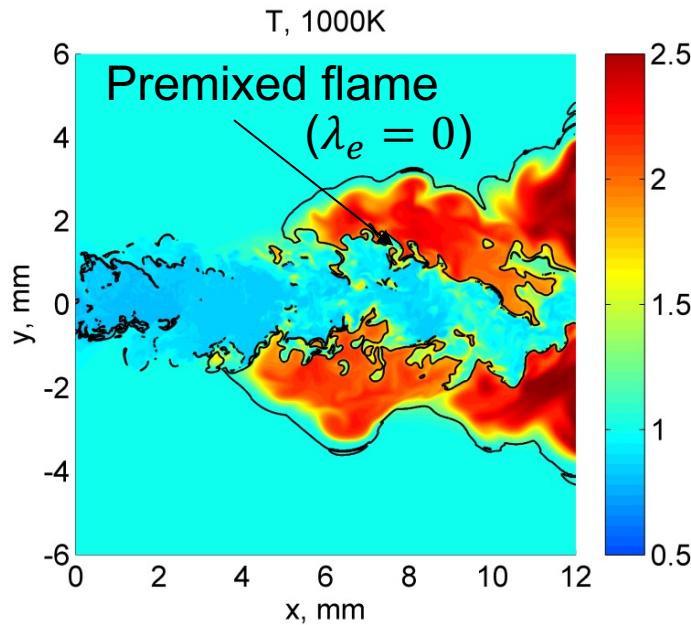
Slaughter et al. 2015



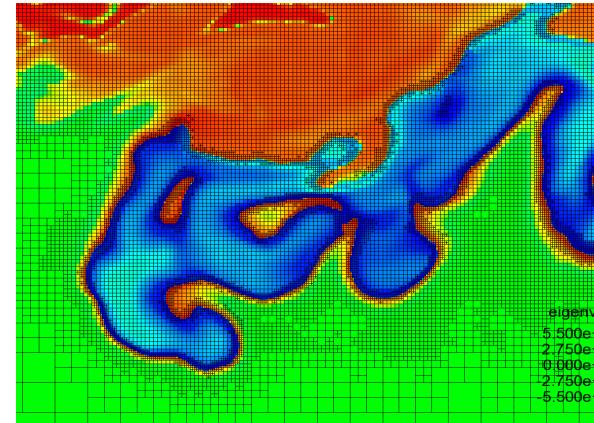
Dependence Graph of S3D

In-Situ Chemical Explosive Mode Analytics (CEMA)

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

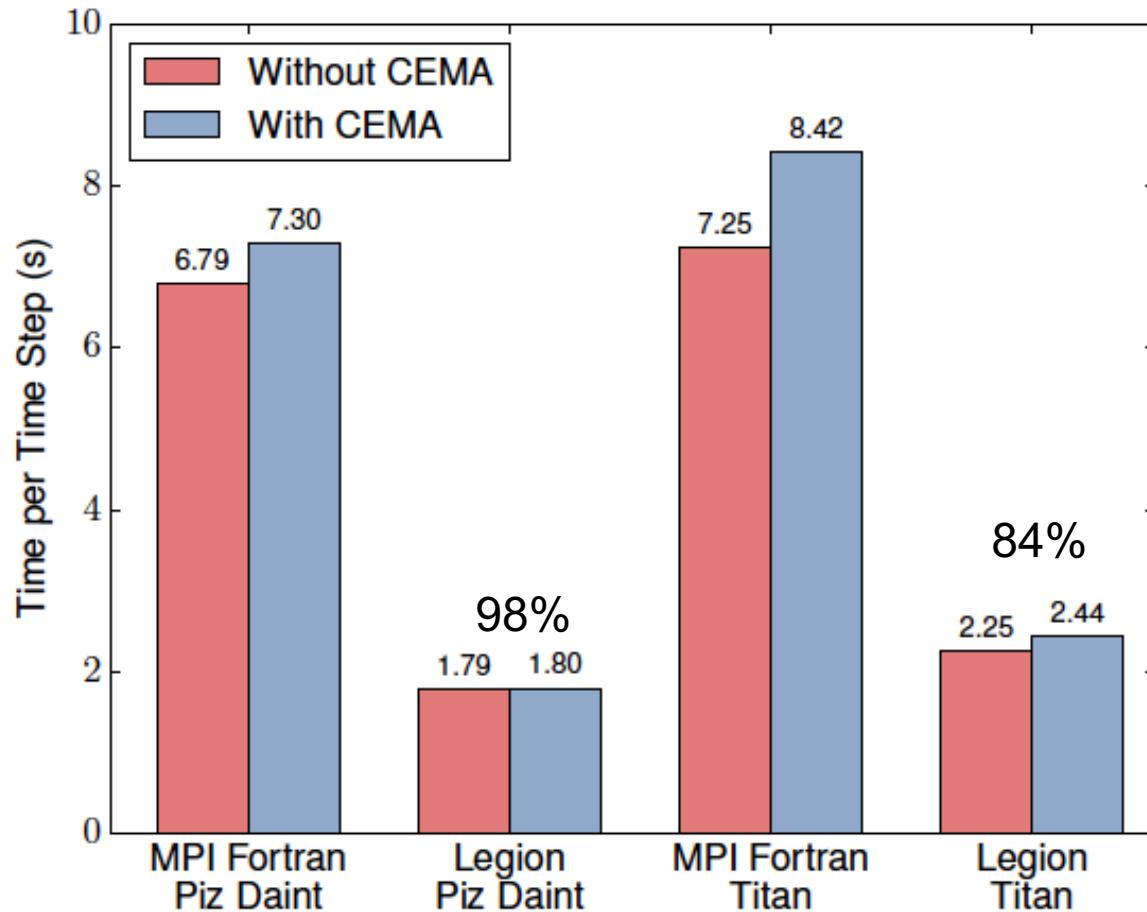


CEMA-based AMR
to capture premixed
fronts ($\lambda_e = 0$)



- 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)



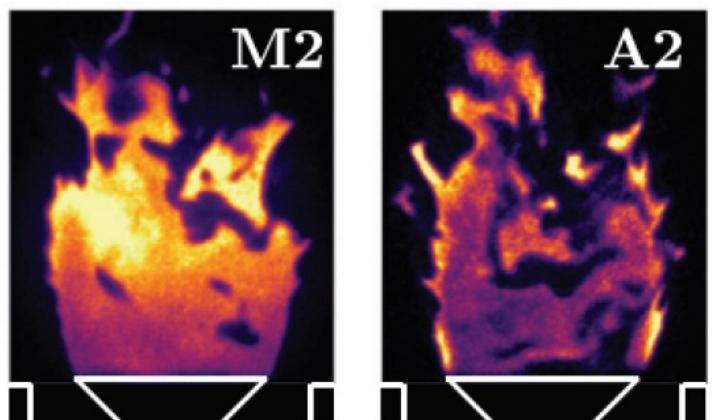
In situ Chemical Explosive Mode Analysis (CEMA) within the S3D Combustion Application – analysis results drive application parameters dynamically.

Reduced overhead of CEMA by a factor of 10 via adaptive/dynamic scheduling of analysis operations (**overhead now less than 2% of overall execution time**).

Runtime system analyzes and allows mapping of dynamic application workloads – e.g. infrequent, changing and data-dependent analysis and visualization operations.

Motivation - Ammonia Combustion

- Ammonia has the potential to be an alternative *zero-carbon* fuel for green long-haul shipping and electricity generation (Kobayashi et al., PROCI, 2019)
- Neat ammonia has a low reactivity compared to, e.g., natural gas (CH_4), which can be improved by adding hydrogen or partial cracking of ammonia to hydrogen and nitrogen, blend can be optimized to match unstrained laminar flame behavior of natural gas



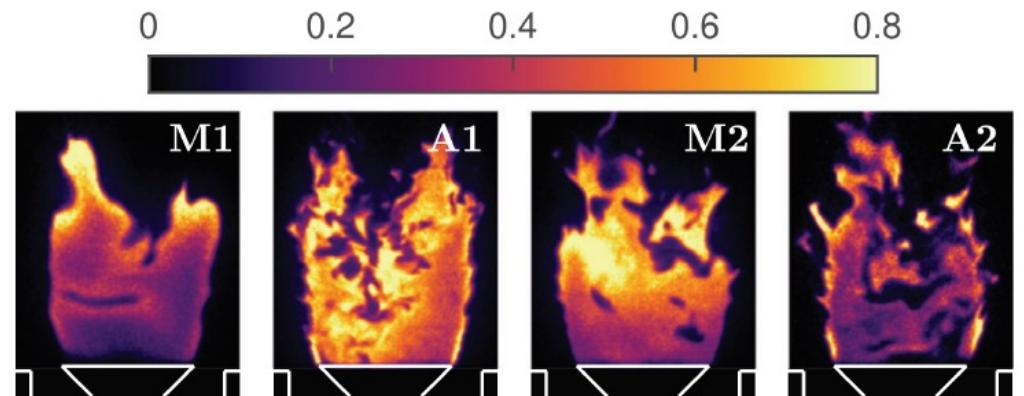
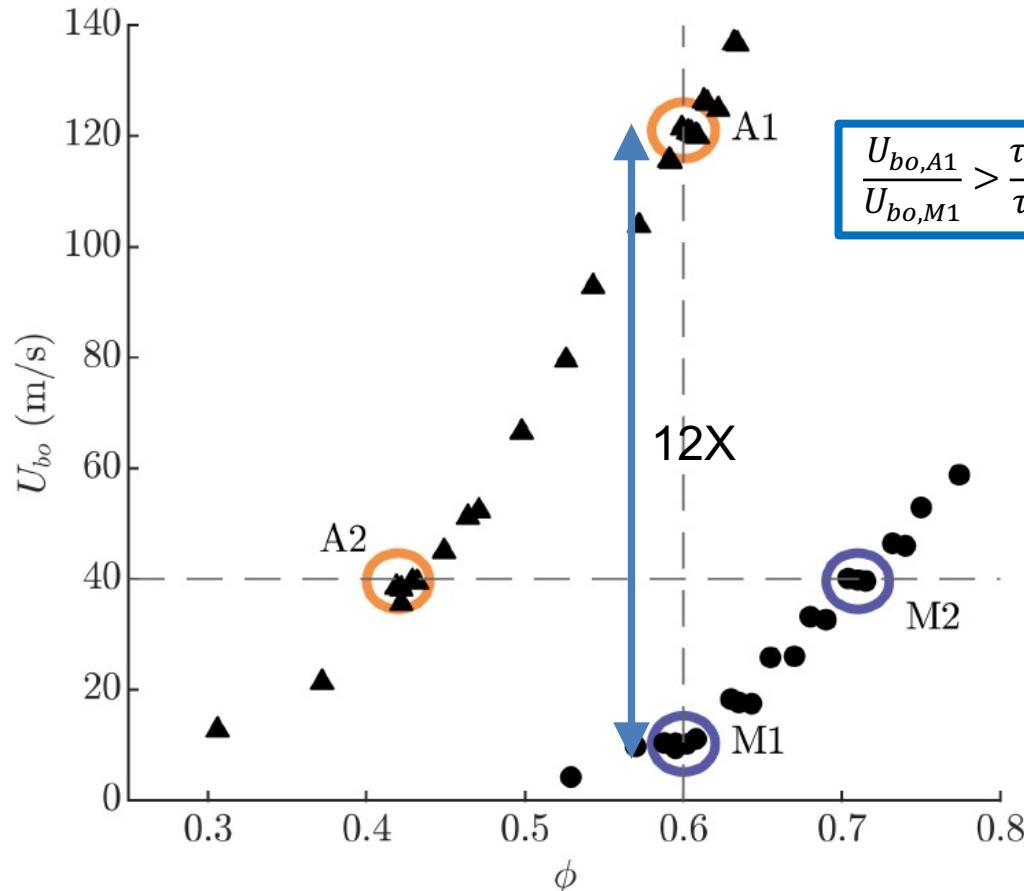
OH PLIF of $\text{NH}_3/\text{H}_2/\text{N}_2$ -air (A2) and methane-air (M2) flames (Wiseman et al., PROCI, 2021)

→ While $\text{NH}_3/\text{H}_2/\text{N}_2$ -air mixtures can be optimized to have unstrained flame properties of CH_4 -air, the turbulent flame behavior can differ significantly

→ Use Direct Numerical Simulation (DNS) of premixed $\text{NH}_3/\text{H}_2/\text{N}_2$ -air flames (as potential natural gas replacement) to elucidate combustion and emission characteristics, in particular at elevated pressures

Experimental Results

Blow-out curves for NH₃/H₂/N₂-air (triangle) and CH₄-air (circle)

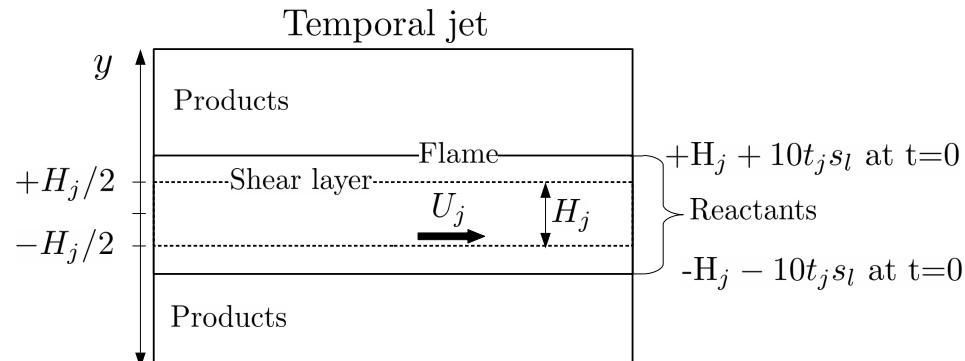


- Lean NH₃/H₂/N₂-air flames are clearly more resilient to blow-out than nominally equivalent CH₄-air flames
- Blow-out velocity is different by one order of magnitude at same ϕ
- At same inflow velocity, much leaner NH₃/H₂/N₂-air flames can be stabilized

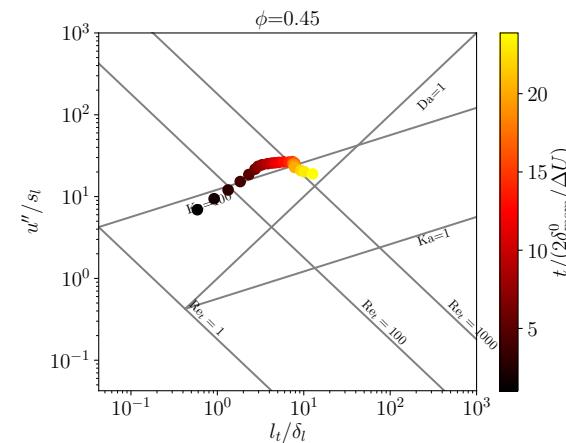
DNS Temporal Slot Jet Configuration

DNS of NH₃/H₂/N₂-air (40%/45%/15%) and CH₄-air:

- 750 K pre-heat temperature, 1 atm, $\phi=0.45$
- $Re_j=13,800$ (NH₃/H₂/N₂), 14,800 (CH₄), same domain size and velocity for both cases
- $Da_j=0.08$ for both cases
- Short chemical kinetics mechanism for H₂/NH₃ combustion in air, derived from San Diego mechanism
(19 species, 63 elementary steps)¹
- Short CH₄-air mechanism (16 species)²



Central jet within reactants,
flame on both sides (in y
direction)

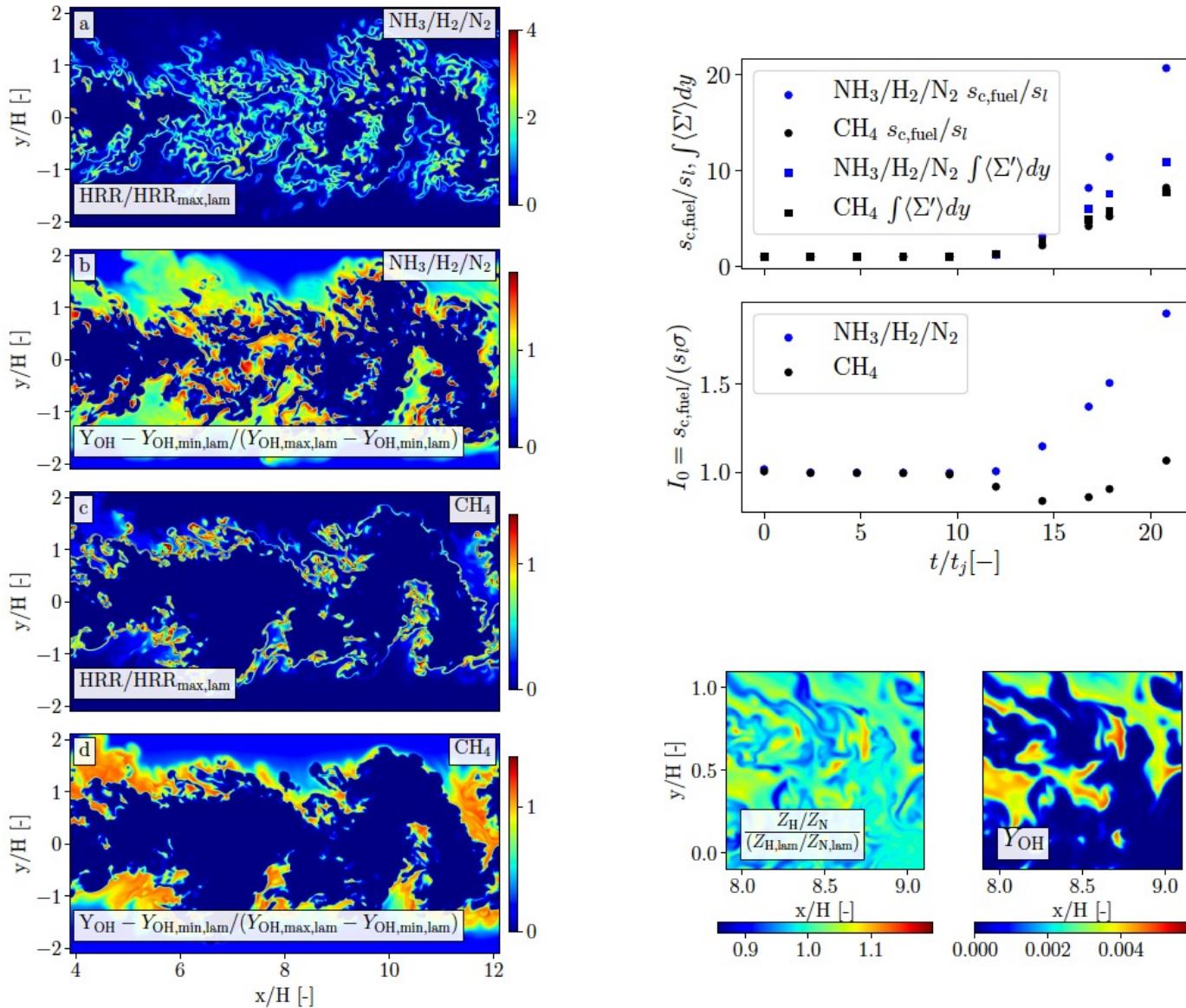


DNS close to border of BRZ and TRZ
regimes
(regime diagram computed at y location
of maximum Re_t)

¹Jiang et al, “An updated short chemical-kinetic nitrogen mechanism for carbon-free combustion applications”, *Int J Energy Res*, vol. 44, pp.795-810 (2020).

²Sooke & Giovangigli, ”Reduced Kinetic Mechanisms and Asymptotic Approximations for Methane-Air Flames”, Springer, pp. 1–28 (1991).

$\text{NH}_3/\text{H}_2/\text{N}_2$ -air vs. CH_4 -air at $\phi=0.45$



- Faster flame surface generation, more intense burning under turbulent conditions (same laminar properties, Da_{jet})
- Main difference affecting turbulent flames: $\text{NH}_3/\text{H}_2/\text{N}_2$ -air shows preferential diffusion effects
- Preferential diffusion leads to super-adiabaticity

Conclusions

- A joint experimental and numerical study was conducted of the blow-out behaviour of $\text{NH}_3/\text{H}_2/\text{N}_2$ -air flames, blended such that the flame exhibits similar premixed, unstretched laminar flame properties as lean methane-air flames
- In the experiment, blow-out curves for the ammonia blend and methane-air flames were measured in an axisymmetric, unconfined, bluff-body stabilized burner, showing an order of magnitude difference in blowout velocity
- DNS of a slot jet configuration revealed that the $\text{NH}_3/\text{H}_2/\text{N}_2$ -air flame exhibits strongly enhanced heat release rates compared to a methane-air flame and points towards preferential diffusion of hydrogen as the main reason for increased burning rates

Pressure Effects on Turbulent Premixed Lean Ammonia/Hydrogen Flames

Martin Rieth², Andrea Gruber³, Myoungkyu Lee², Forman Williams⁴, Jacqueline Chen²

Visualization: Tyson Neuroth¹, Qi Wu¹, Kwan-Liu Ma¹

¹ University of California, Davis, ²Sandia National Laboratories, ³SINTEF Energy Research, ⁴University of California at San Diego

Motivation

High Pressure Premixed Combustion

- Gas turbine combustors operate at ~20-30 atm
- Premixed combustion at pressurized conditions is not fully understood and studied to a limited extent due to cost
- Previous studies: larger normalized turbulent burning velocity (e.g., Kobayashi et al., 2000; Venkateswaran et al., 2014)

Ammonia/hydrogen/nitrogen combustion

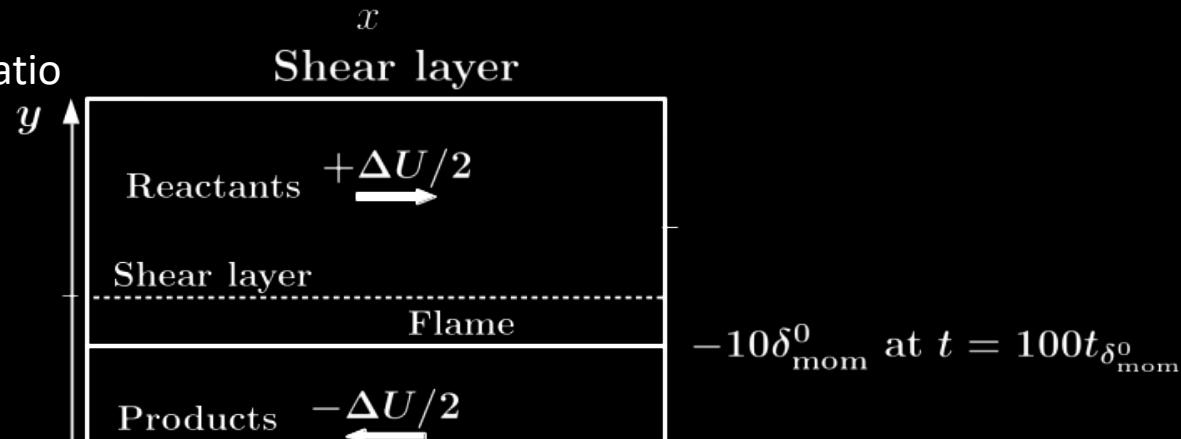
- Ammonia (NH₃) is a promising energy carrier for zero-carbon combustion
- Blends of NH₃/H₂/N₂ can be optimized to have unstrained laminar flame behavior close to that of natural gas
- However, lean turbulent combustion behavior of NH₃/H₂/N₂ differs to that of natural gas (Wiseman et al., 2021) due to the thermo-diffusive nature → not fully understood yet, especially at elevated pressure

Pressure effects on ammonia/hydrogen premixed flames: direct numerical simulations in a temporal planar shear layer configuration

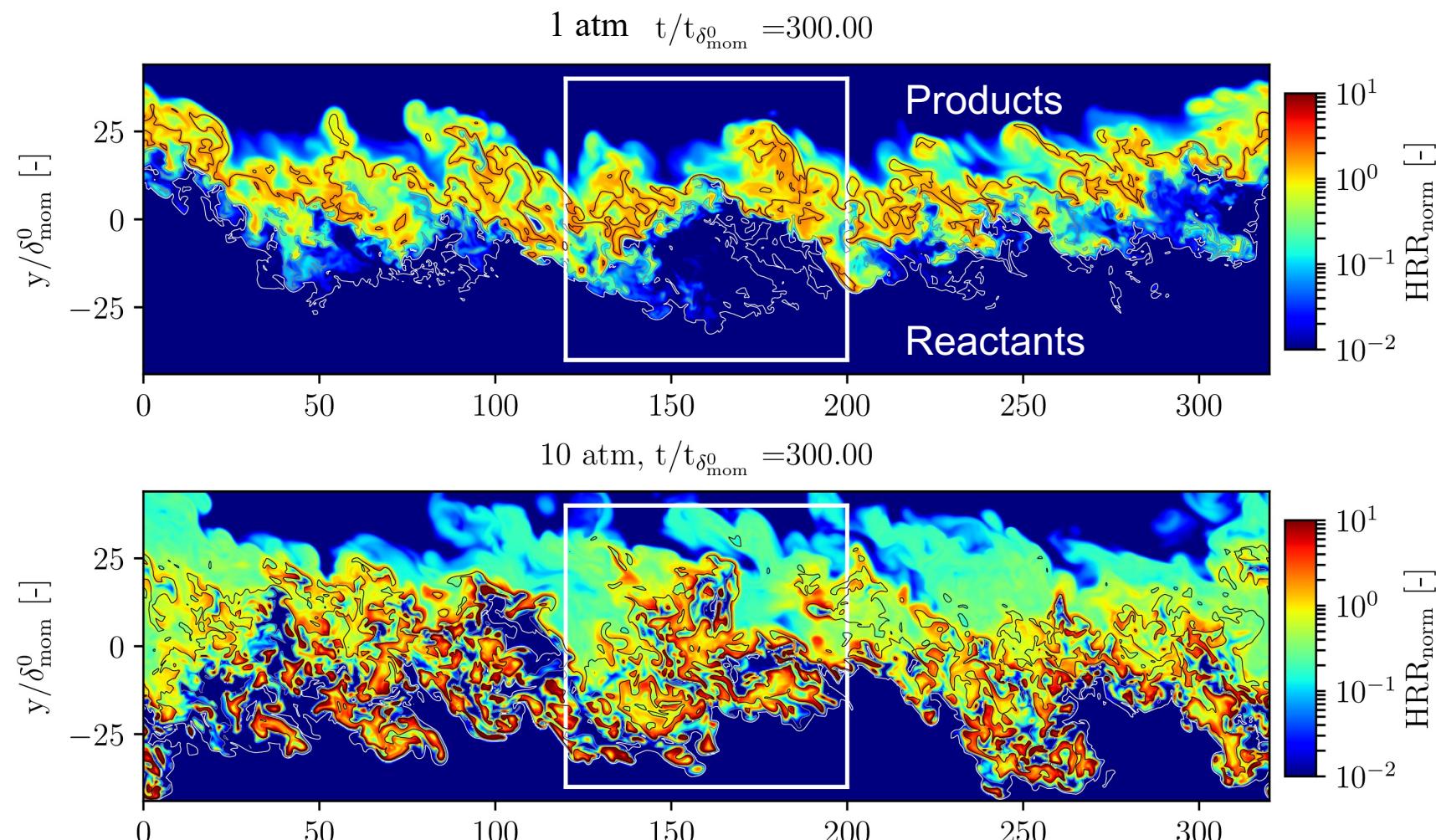
Simulation Parameters

- Lean premixed NH₃/H₂/N₂-air (40%/45%/15% vol) with equivalence ratio of 0.45 at **1 and 10 atm**
- Reactants are preheated to 750 K
- Flames are nominally in the broken reaction zone regime (Karlovitz # (Ka)>600, turbulent Re # (Re_t)>1000)
- Simulations are designed such that normalized parameters (Re_t, Ka, Damköhler #) are consistent between 1 and 10 atm
- Growing grid size with 11 B grid points on the final grid
- 19 species chemical mechanism (Jiang et al., 2020)
- DNS using S3D-Legion run on OLCF's 200 Pflop Summit supercomputer on ~1000 nodes using a DOE INCITE allocation

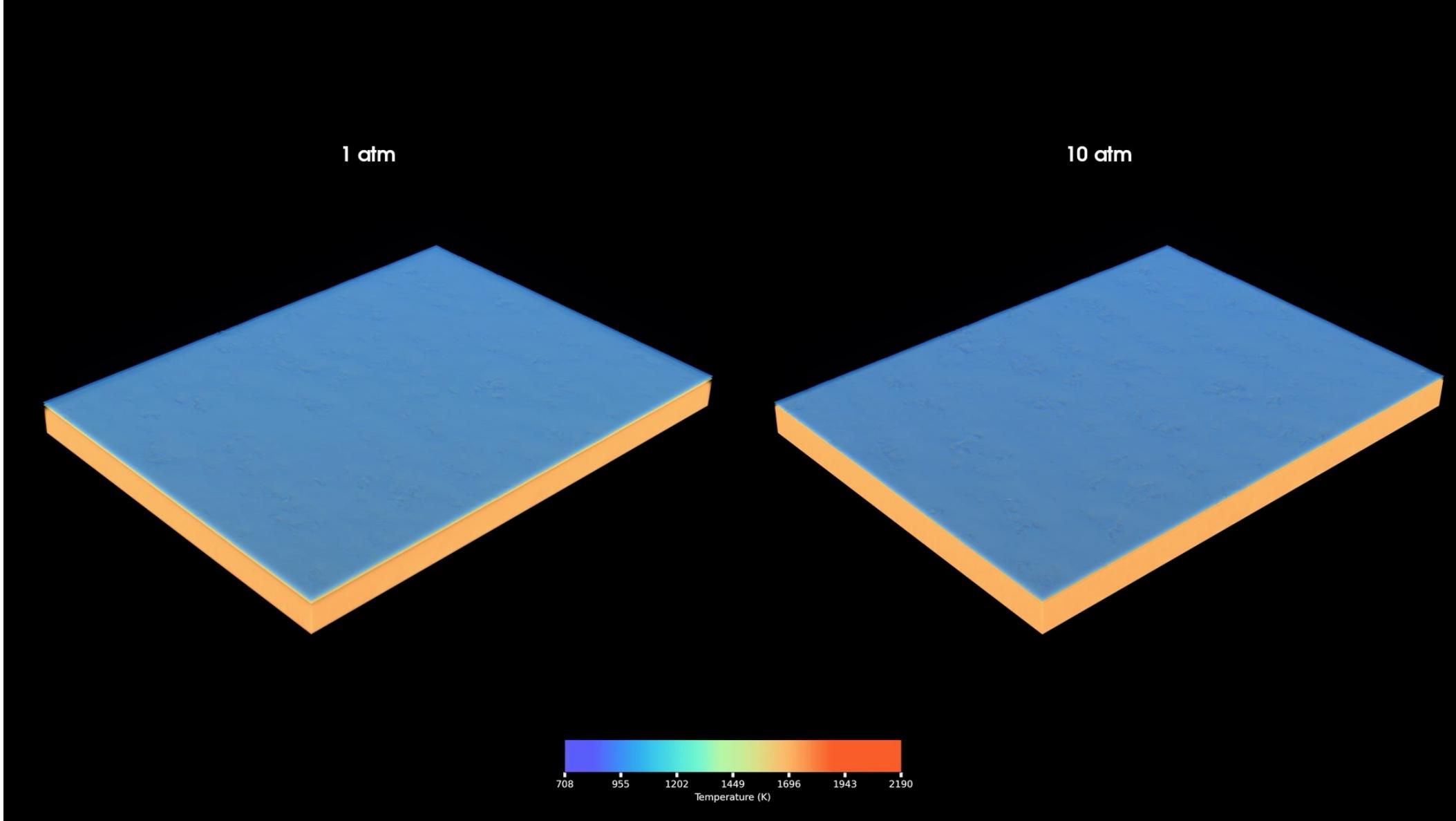
Simulation setup



Heat release rate from NH₃/H₂/N₂/air premixed flame in turbulent mixing layer at 1 and 10 atm



Iso-lines correspond to temperatures of 800 (white), 1000(grey) and 1500 K (black)

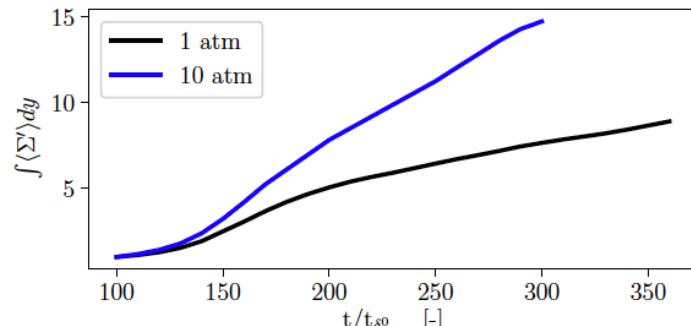


- Strong shear-driven turbulence wrinkles and disrupts the flame front
- More wrinkling and cellular structures appear at 10 atm, disrupted preheat zone at 1 atm
- Strong super-adiabaticity at 10 atm, larger fluctuations in equivalence ratio

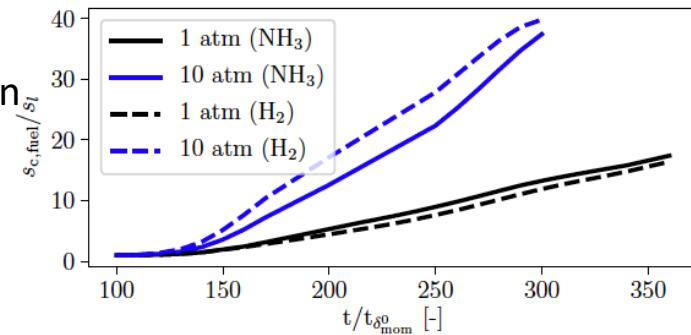
Thermo-diffusive instabilities and preferential diffusion

Flame Surface Area and Burning Rate

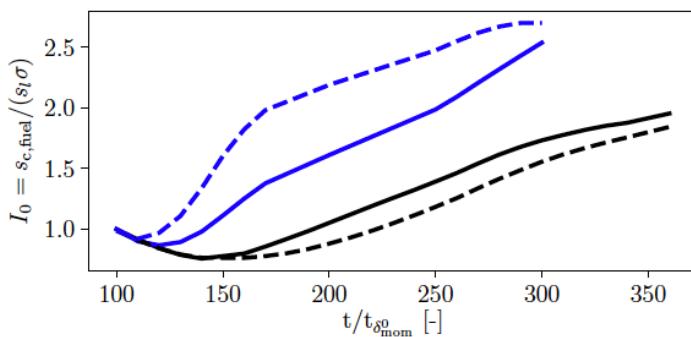
Flame surface density



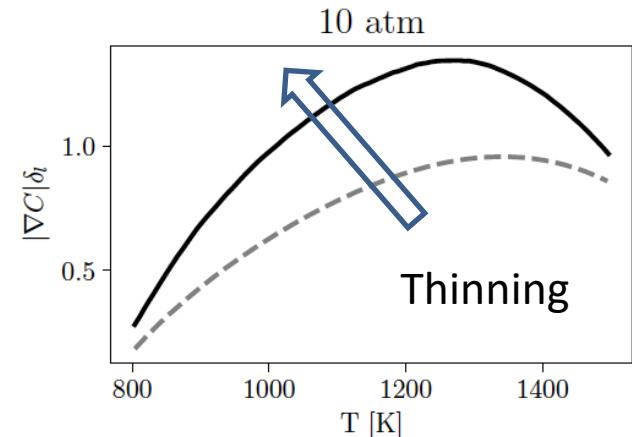
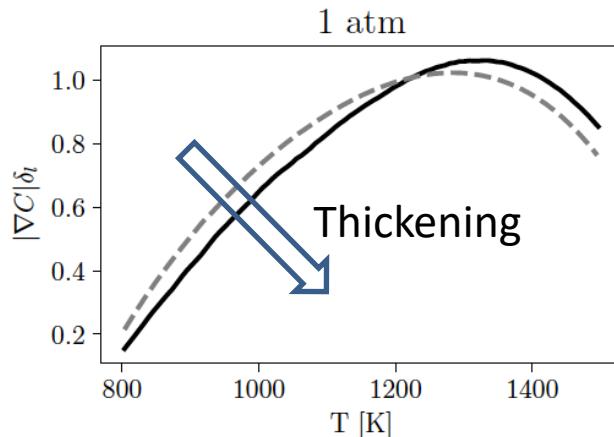
Fuel consumption speed



Burning Intensity



Flame thickness

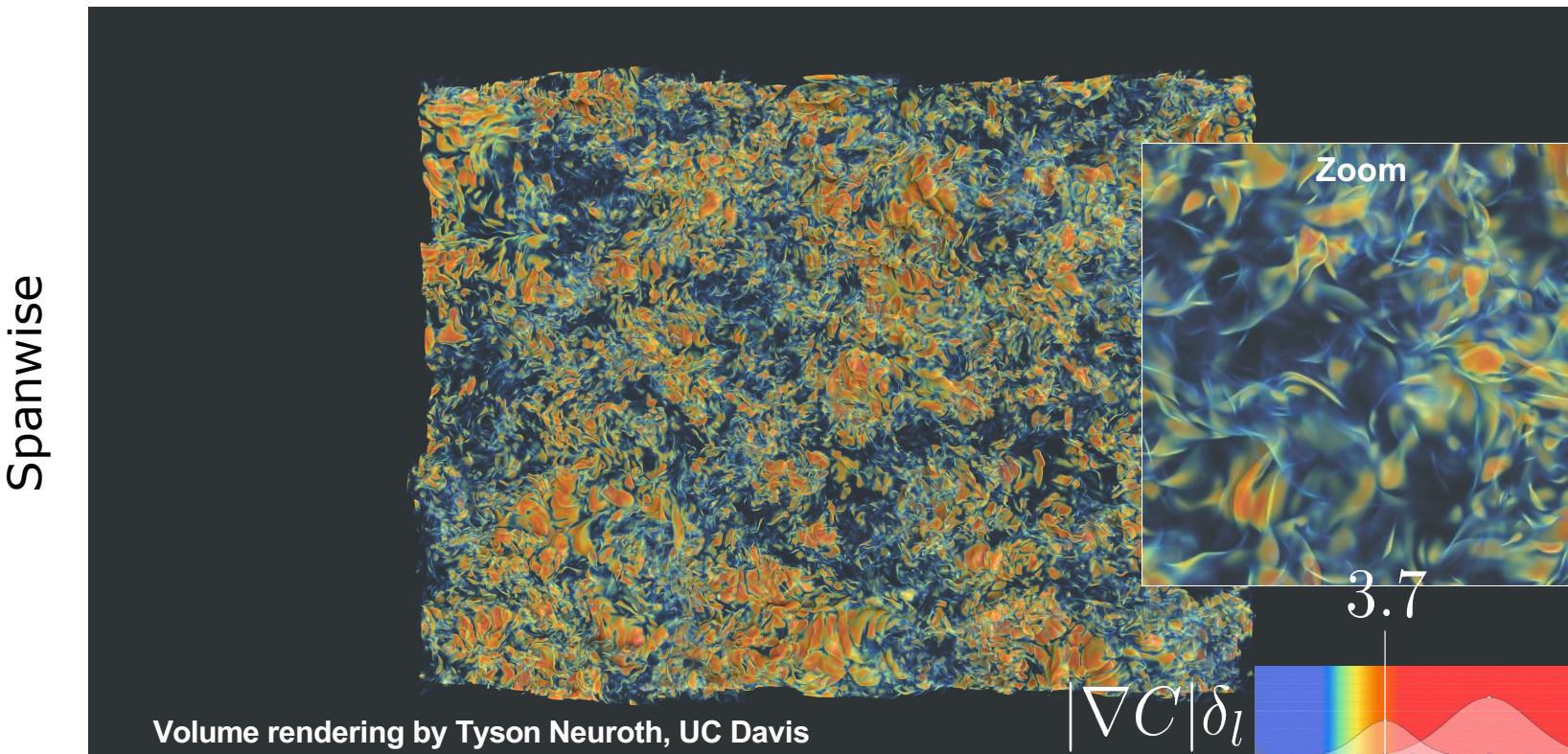


Black lines represent DNS solution at $t/t_{\delta_{mom}^0} = 300$. Grey dashed lines represent laminar flame solution.

- Faster increase of flame surface density ($\int \langle \Sigma' \rangle dy$), overall fuel consumption speed ($s_{c,fuel}/s_l$) and burning intensity (I_0)
- Thinner flames at 10 atm (larger $|\nabla C| \delta_l$)

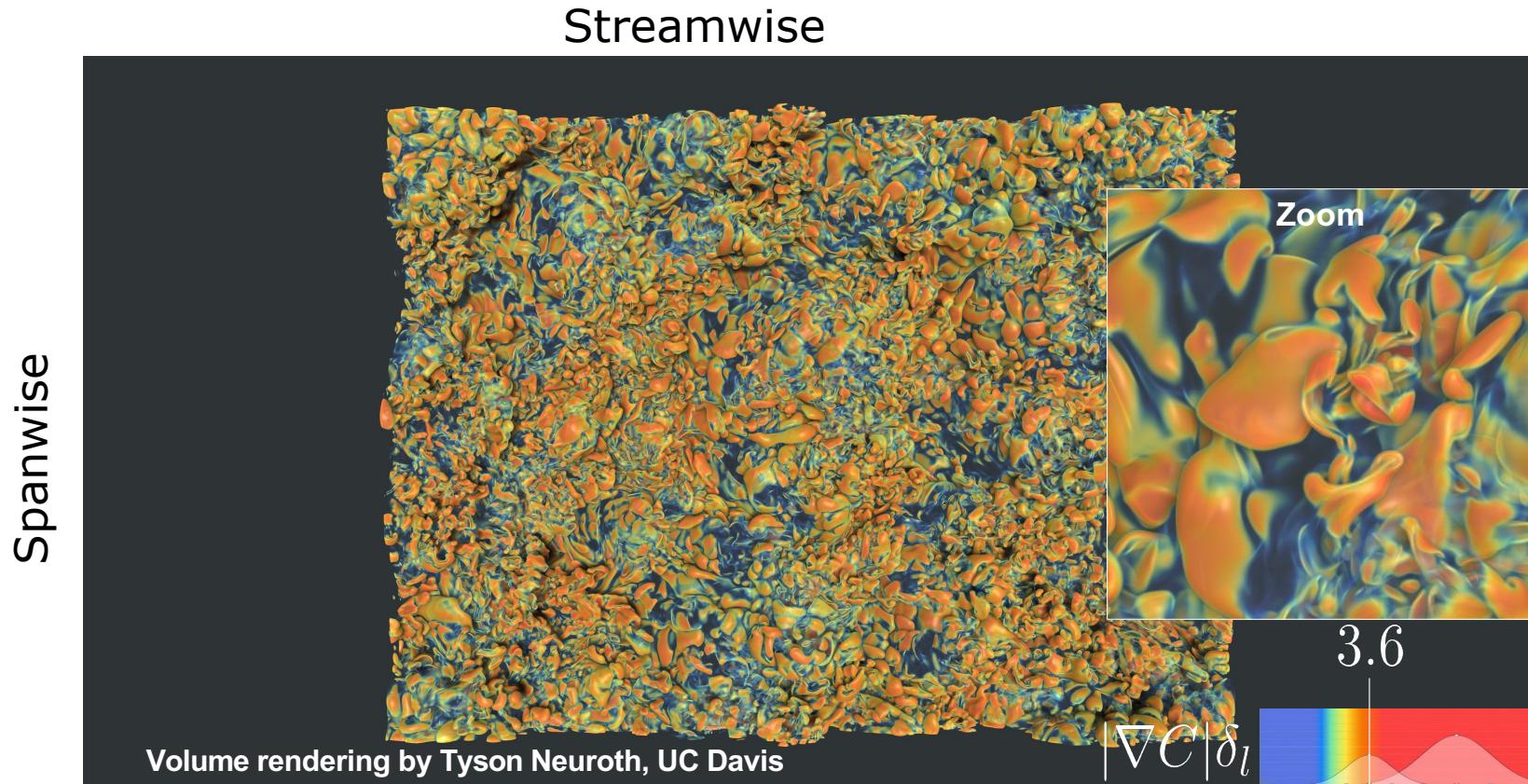
Volume Rendering of Fine-Grained Flame Surface Density $|\nabla C|$ at 1 atm ($t/t_{\delta_0} = 300$)

Streamwise



At 1 atm, turbulence disrupts the flame structure to a large extent, but some cellular flame structures can be observed

Volume Rendering of Fine-Grained Flame Surface Density $|\nabla C|$ at 10 atm ($t/t_{\delta_0} = 300$)



At 10 atm, the flame is dominated by cellular flame structures, indicative of thermo-diffusive effects, $|\nabla C|$ is generally larger than at 1 atm and flame features are smaller

Fractal Analysis of Turbulent Flames

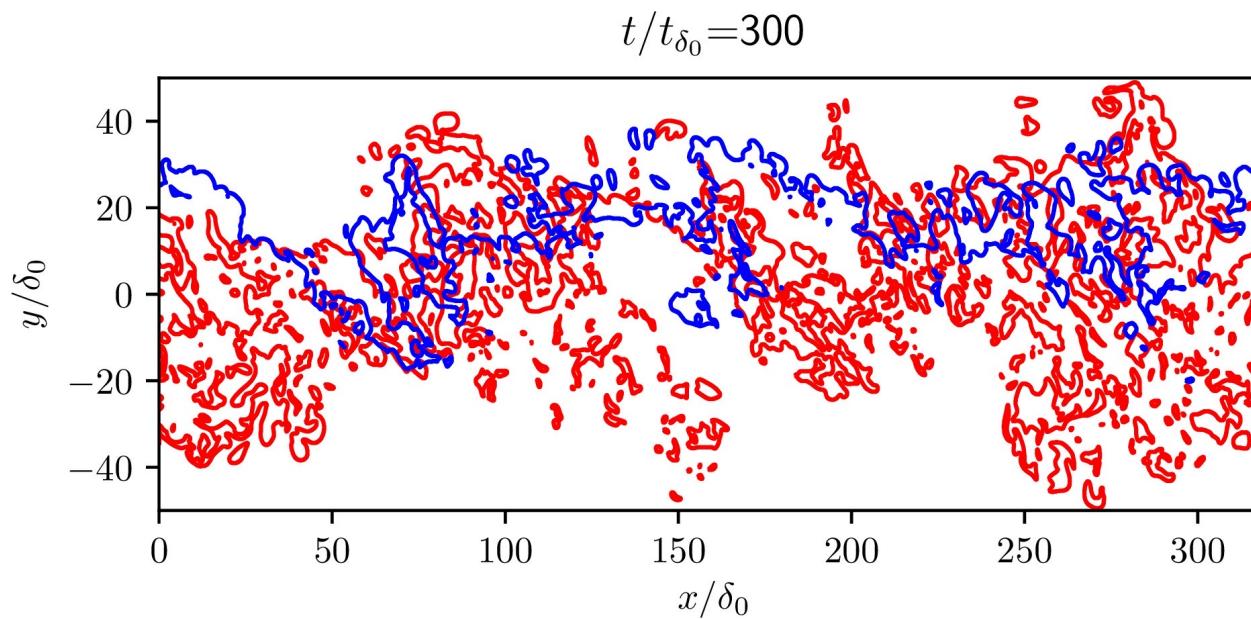
Background

- Chatakonda et al. (C&F, 2013) analyzed the fractal characteristics of low Damkohler premixed flames, found upper limit of $8/3$ (different to previous theoretically derived maximum of $7/3$ by Kerstein (CST, 1988))
- Rasool et al. (C&F, 2021) compared weakly turbulent flames (high Da, low Ka) at different Lewis numbers and pressures, found that fractal dimension increases for decreasing Lewis number and increasing pressure, approaching a value of $7/3$
- Unstable (laminar) spherical flames show varying fractal dimensions, but typically stay below $7/3$ (Cai et al, C&F 2016; Liu et al., JFM, 2021), fractal dimension of $7/3$ is a measure for self-turbulization

Procedure to obtain fractal dimensions (FD):

- Define flame surface (definition is important as will be shown)
- Box counting algorithm: count number of boxes to cover flame surface for different box sizes → obtain FD from slope of number of boxes vs. box size

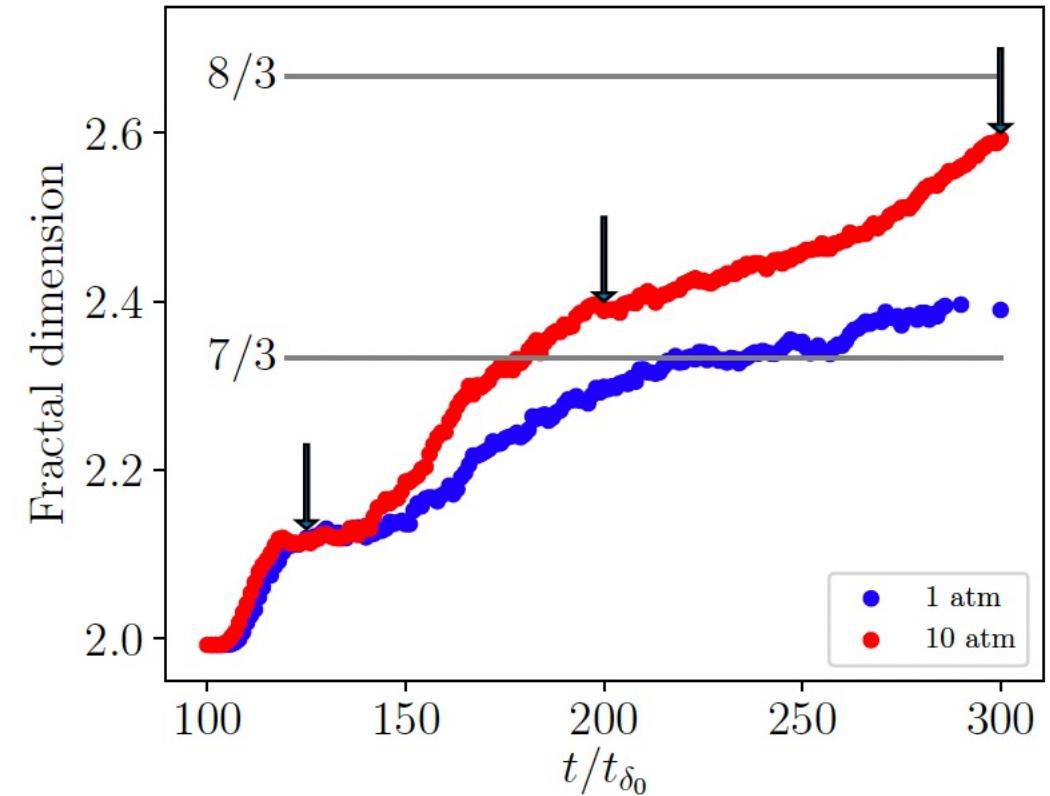
Flame Surface at $t/t_{\delta_0} = 300$ and Fractal Dimension (FD) vs. Time



1atm 10atm (flame surface based on H₂O)

Flame surface corresponds to H₂O mass fraction

value at maximum HRR in unstrained laminar flame



- FD increases faster and reaches higher levels at elevated pressure conditions
- Major difference in behavior: late increase in slope for 10 atm (onset of cellular instabilities)
- Thermo-diffusive instabilities clearly affect FD and models need to account for turbulence and instability effects

Performance of time-dependent reduced-order modeling of transient combustion phenomena

Swapnil Desai¹, Jacqueline H. Chen¹, Kisung Jung¹, Seshu Yamajala², Hessam Babaee³

¹Sandia National Laboratories

²SLAC

³University of Pittsburgh

Motivation

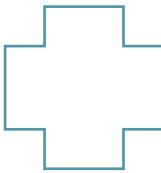
Direct Numerical Simulation (DNS)

Advantages:

- Full access to time resolved 3D fields

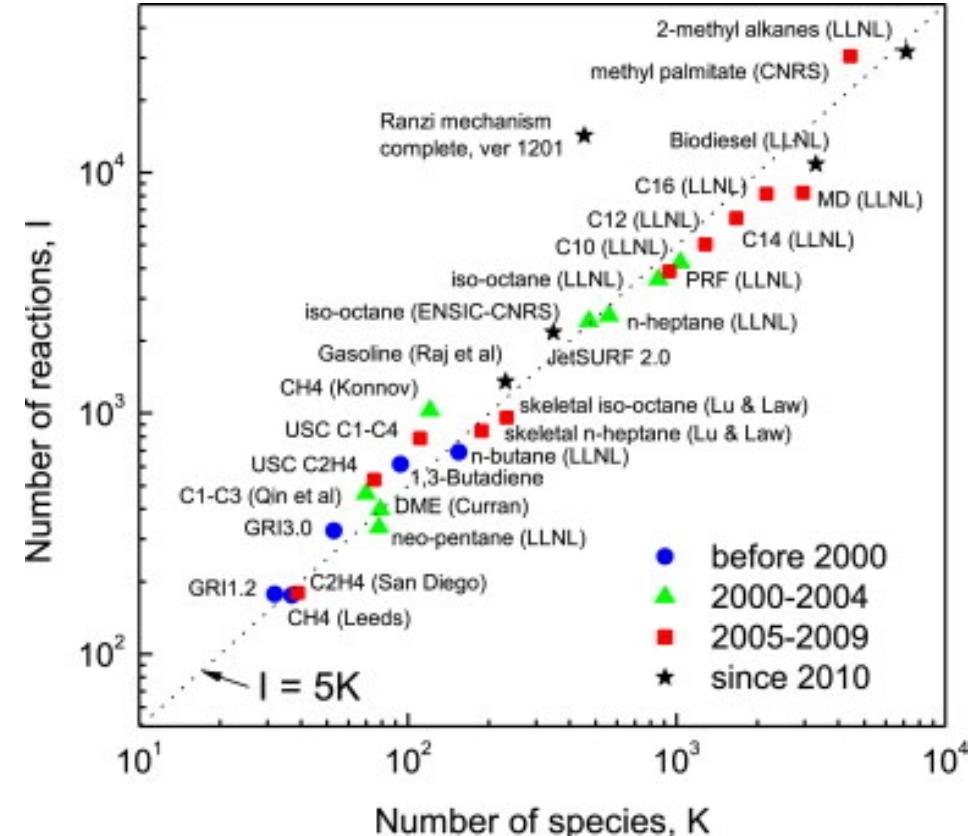
Disadvantages:

- Huge computing and memory requirements



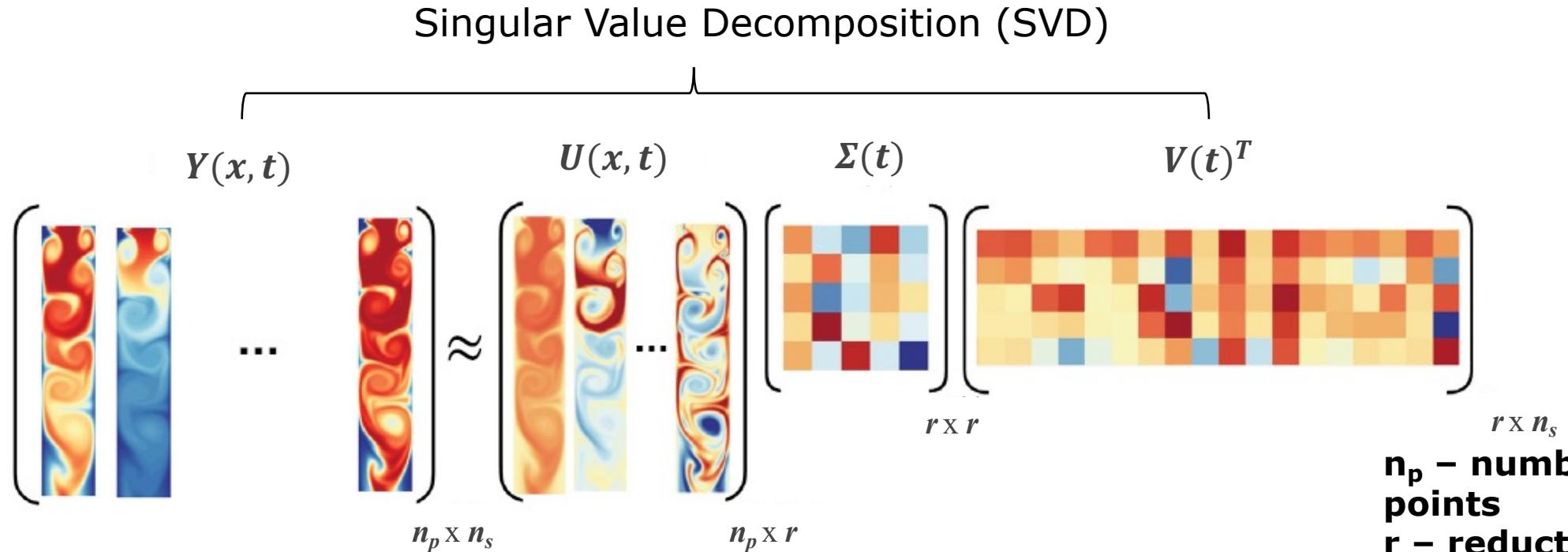
Solutions:

- Use of skeletal / reduced kinetic mechanisms
 - Mechanism size for gasoline / diesel surrogates still upwards of 100 species and 1000 reactions
- Principal component analysis (PCA) based reduced-order modeling (ROM)
 - Need for high fidelity training data



1: Egolfopoulos et al., PECS, 2014

Dynamically bi-orthonormal (DBO) decomposition based ROM



Idea: Obtain on-the-fly low-rank decomposition of species transport equation^{1,2}

Advantages:

- No need to generate training data
- Extract instantaneous correlations between different species on the fly and directly from the species transport equation
- No need to store the entire species vector
- Potential to scale linearly w.r.t. data size and low-rank- r without requiring to solve large scale optimization problem

n_p – number of grid points
 r – reduction size
 n_s - number of species ($r \ll n_s$), includes the bath gas

1: Patil et al., JCP 2020

2: D. Ramezanian et al., Comp. Met. Appl. Mech. & Eng., 2021

DBO: Math

$$\frac{\partial Y_i}{\partial t} = -\frac{1}{\rho} \left(u \frac{\partial Y_i}{\partial x} + v \frac{\partial Y_i}{\partial y} + w \frac{\partial Y_i}{\partial z} \right) - \frac{1}{\rho} \left(\frac{\partial J_{i,x}}{\partial x} + \frac{\partial J_{i,y}}{\partial y} + \frac{\partial J_{i,z}}{\partial z} \right) + \frac{W_i \dot{\omega}_i}{\rho} \quad (\text{Modified Governing equation})$$

Evolve the governing equation for few time steps (~ 1000) with DNS so that rank (i.e. r) based on instantaneous-PCA increases and then switch to DBO

$$J_{i,\alpha} = -\rho D_i^{mix} \left[\nabla_\alpha Y_i - Y_i W \sum_{j=1}^{N_s} \frac{\nabla_\alpha Y_j}{W_j} \right]$$

$$\frac{\partial U}{\partial t} = \prod_{\perp U} \left[- \left(u \frac{\partial U}{\partial x} + v \frac{\partial U}{\partial y} + w \frac{\partial U}{\partial z} \right) + \left(\frac{\partial J_{i,x} V}{\partial x} + \frac{\partial J_{i,y} V}{\partial y} + \frac{\partial J_{i,z} V}{\partial z} \right) \Sigma^{-1} + \frac{W_i \dot{\omega}_i}{\rho} V \Sigma^{-1} \right] \rightarrow PDE$$

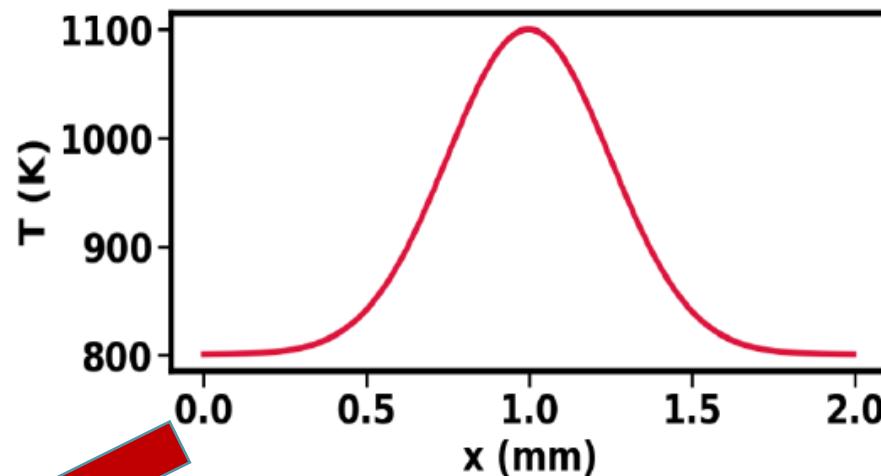
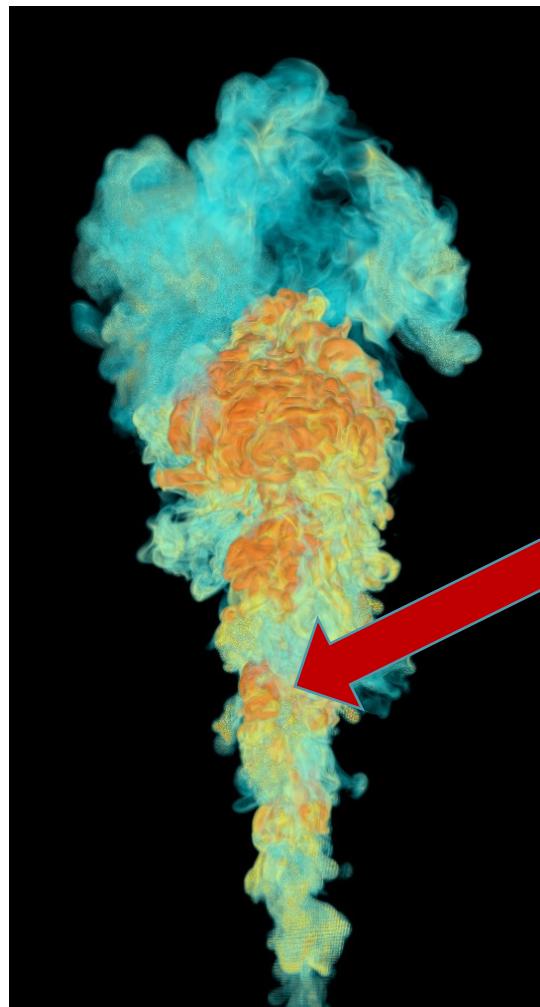
$$\frac{d\Sigma}{dt} = \left\langle U, u \frac{\partial U}{\partial x} + v \frac{\partial U}{\partial y} + w \frac{\partial U}{\partial z} \right\rangle \Sigma + \left\langle U, \frac{\partial J_{i,x} V}{\partial x} + \frac{\partial J_{i,y} V}{\partial y} + \frac{\partial J_{i,z} V}{\partial z} \right\rangle + \left\langle U, \frac{W_i \dot{\omega}_i}{\rho} V \right\rangle \rightarrow ODE$$

$$\frac{dV}{dt} = \prod_{\perp V} \left[\left\langle \frac{\partial J_{i,x}}{\partial x} + \frac{\partial J_{i,y}}{\partial y} + \frac{\partial J_{i,z}}{\partial z}, U \right\rangle + \left\langle \frac{W_i \dot{\omega}_i}{\rho}, U \right\rangle \right] \Sigma^{-T} \rightarrow ODE$$

D. Ramezanian et al.,
Comp. Met. Appl.
Mech. & Eng., 2021

$$\prod_{\perp U} f = f - U \langle U, f \rangle \quad \text{and} \quad \prod_{\perp Y} z = z - YY^T z \quad \langle U, f \rangle = \sum_{p=1}^{p=m} matmul(U^T, f), \\ m = \text{number of processors}$$

Canonical test case: 1D hotspot of lean n-heptane/air



Pele DNS of turbulent multi-injection autoignitive diesel jet

$T_{\text{mean}} = 800 \text{ K}$, $T_{\text{peak}} = 1100 \text{ K}$, $P = 50 \text{ bar}$, $\phi = 0.4$

52 species n-heptane air mechanism¹

S3D²: 8th order finite difference operator, 4th order, 6-stage explicit Runge-Kutta time integrator, LAPACK for linear algebra operations

2 micron grid resolution, 1 ns time step size

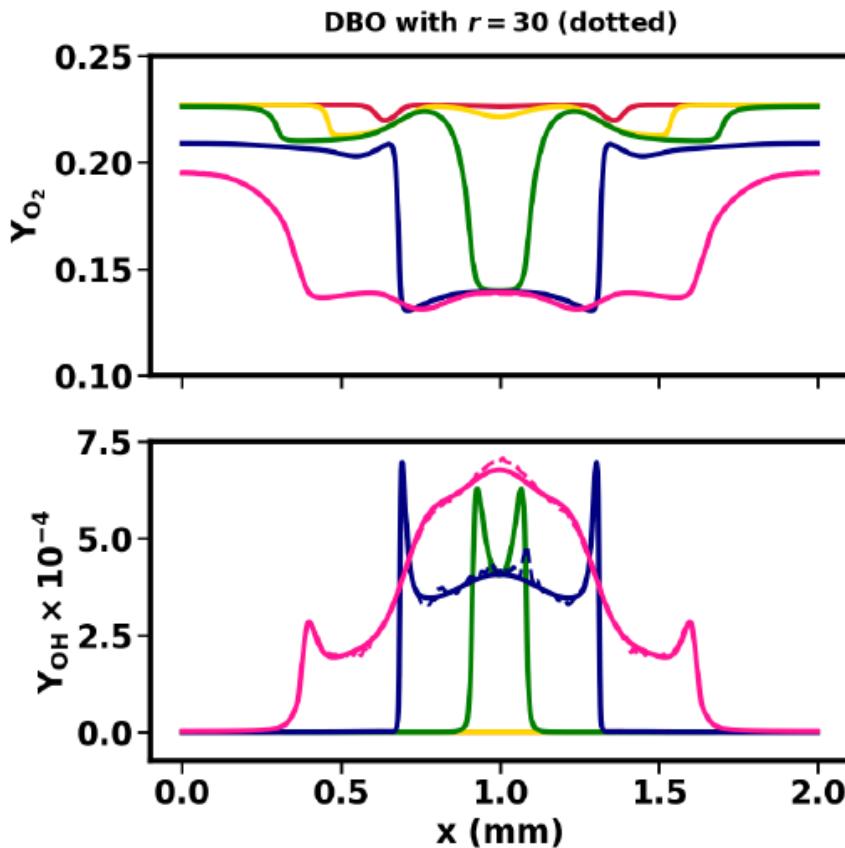
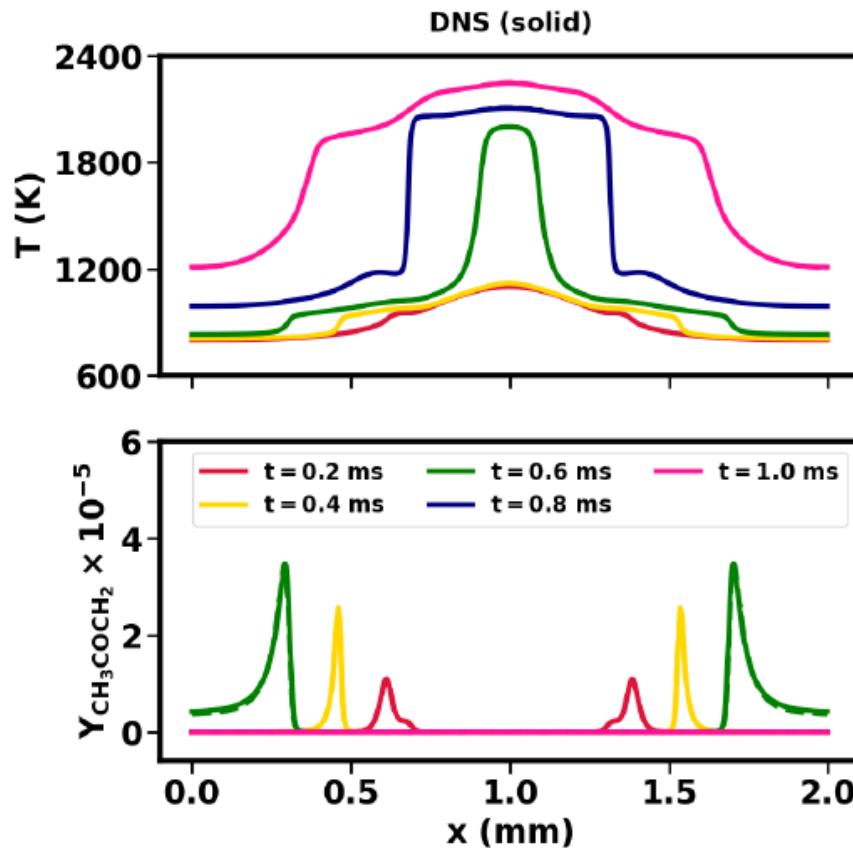
Periodic boundaries at $x = 0$ and $x = 2 \text{ mm}$

DBO started at $t = 0.2 \text{ ms}$ and ran for additional 0.8 ms.

1: Lu et al., Combust. Flame, 2009

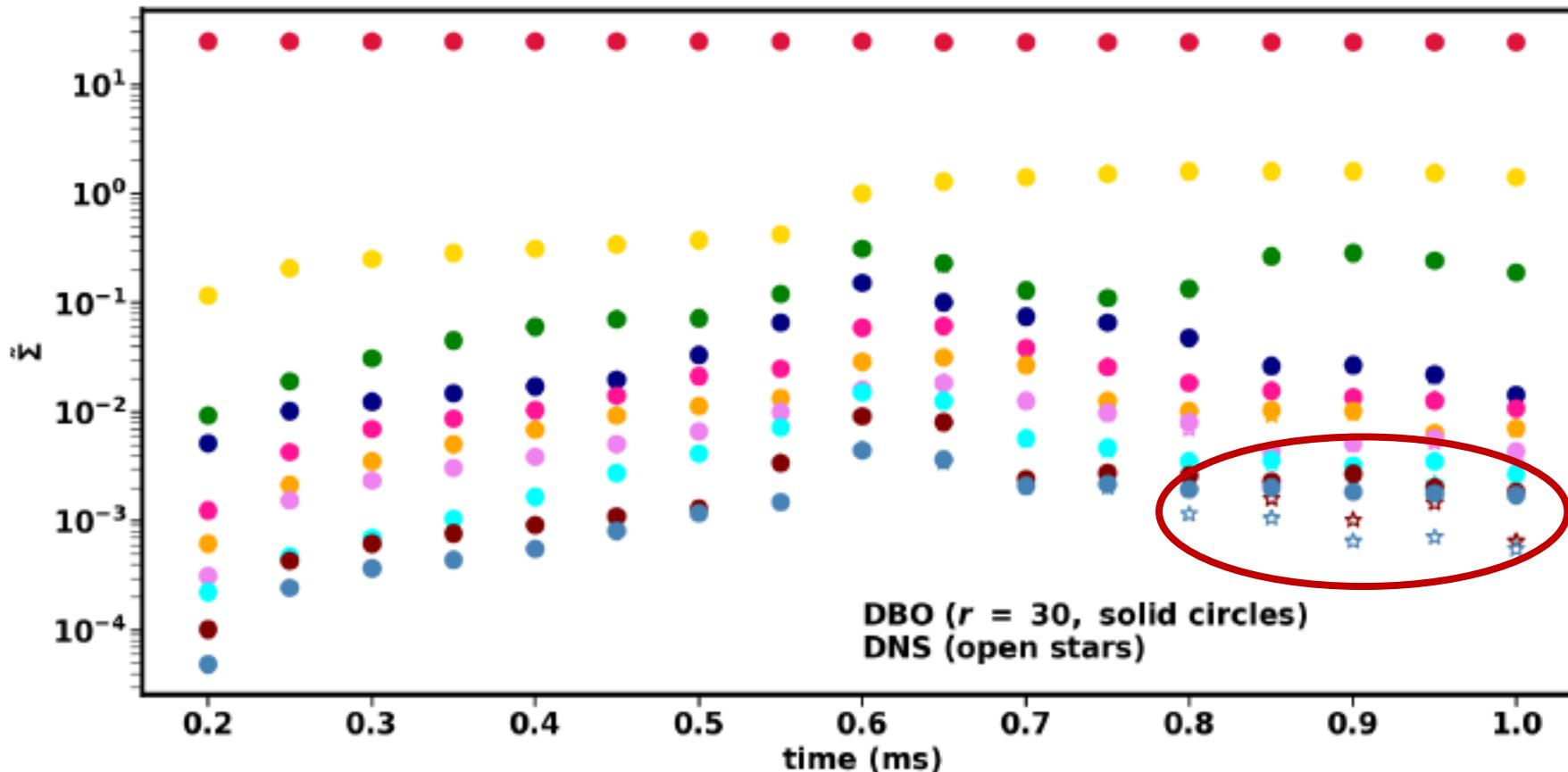
2: Chen et al., Comp. Sci & Disc. 2009.

Transient auto-ignition: DNS versus DBO



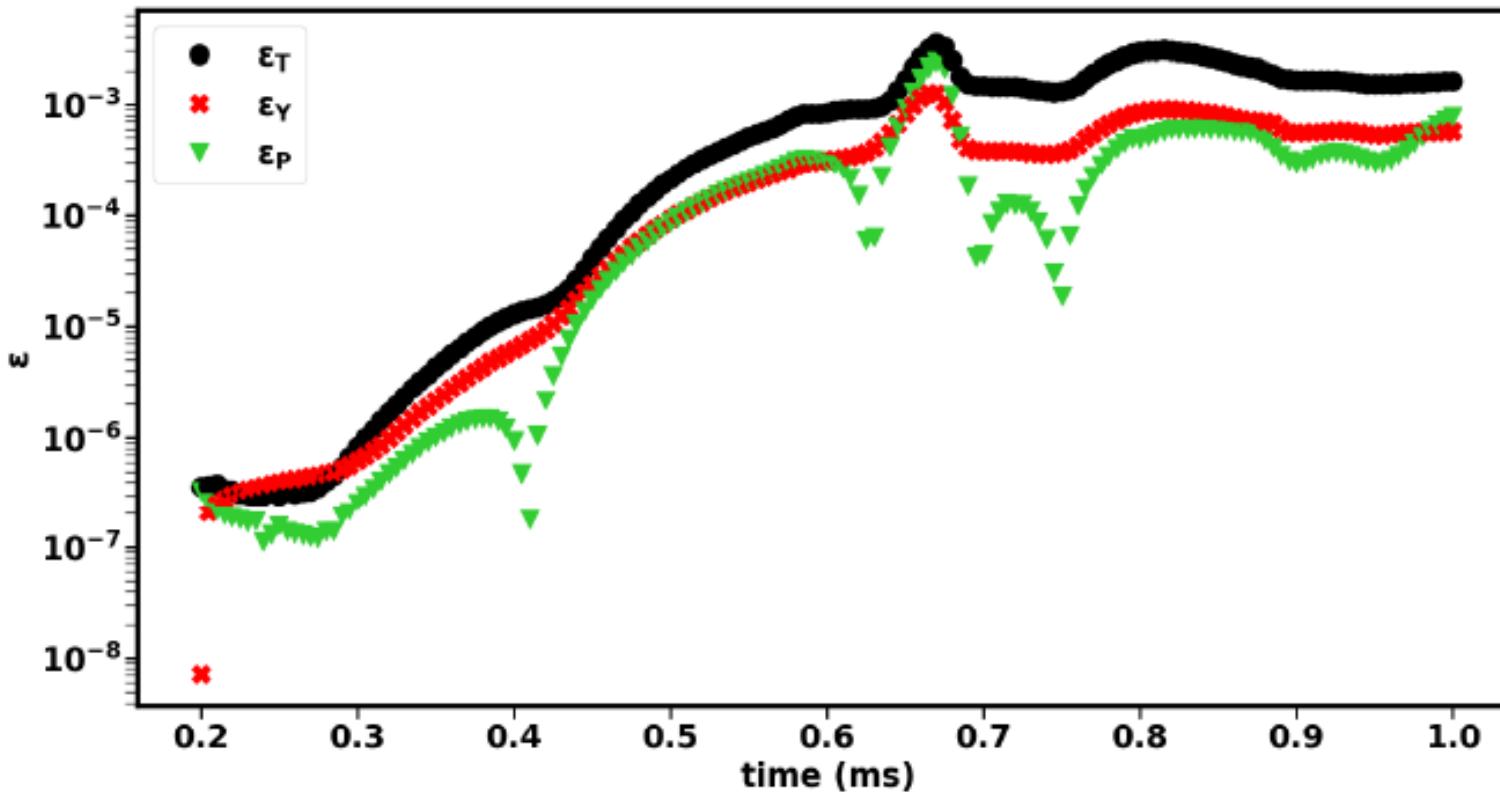
- DBO simulation performed with $r = 30$
- Low temperature chemistry identified by CH_3COCH_2 radical
- High temperature chemistry identified by OH radical
- DBO able to capture the entire transient ignition process: low-temperature ignition \rightarrow cool flame propagation \rightarrow high-temperature ignition \rightarrow hot flame propagation
- Differences in the OH profiles appear around 0.8 ms

Temporal evolution of covariance matrix: DNS (Instantaneous-PCA) versus DBO



- DBO accurately captures first 10 singular values until $t = 0.7$ ms beyond which the accuracy of DBO degrades
- Since $r < n_s$, errors accumulate over time due to lost interactions of DBO modes with unresolved modes
 - Affects the modes with smaller singular values more intensely¹
 - Spurious oscillations appear in mass fraction profiles at later times

DBO approximation error



$$\epsilon(t) = \left\| Y(x,t) - U(x,t)\Sigma(t)V(t)^T \right\|_F / \|Y(x,t)\|_F \quad \left\| \cdot \right\|_F \rightarrow \text{Frobenius Norm}$$



Full rank solution



DBO reconstruction

Conclusions

- DBO based ROM of compressible reacting flow demonstrated to accurately capture strongly transient phenomena involving multiple stages of combustion as observed in a lean n-heptane/air mixture at high pressure and temperature
 - With only 30 modes, ~57% of the total species in the chosen chemical mechanism
 - Without needing high fidelity training data

Future Work

- Perform additional test cases with open/wall boundaries in multiple dimensions and larger mechanisms such as PRF¹ and TPRF-Ethanol²
- Derive DBO equations for fully conserved form of species transport equation
 - Better suited for detonation cases and application of NSCBCs
- Implement sparse sampling for DBO reconstruction in compressed form to reduce cost of reaction source term evaluation

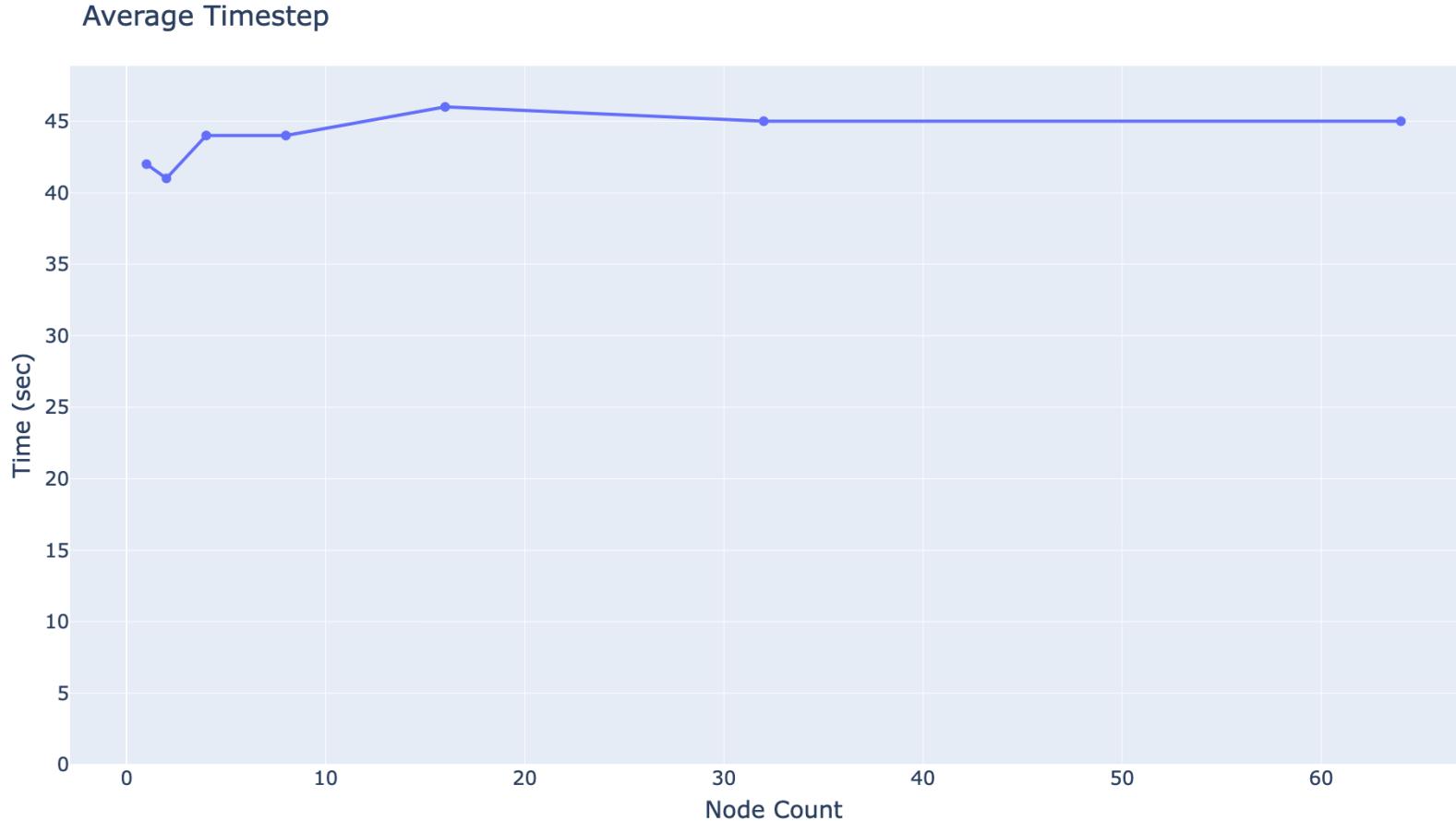
1: Luong et al., Combust. Flame, 2013

2: P. Pal et al., JERT, 2018

Legion S3D-DBO

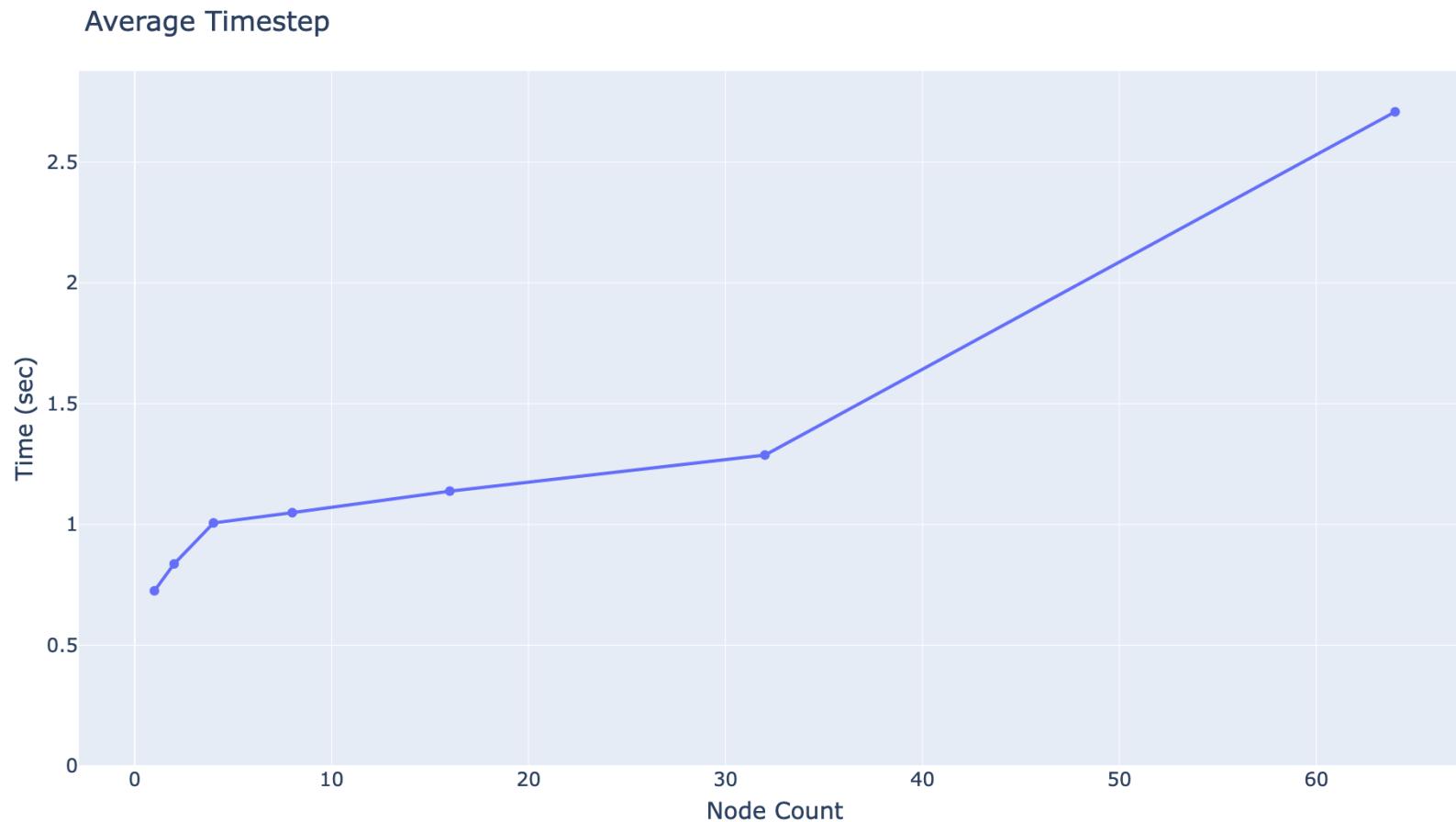
- DBO implementation in S3D ported to Legion/Regent
- All kernels ported to GPU
- Performed weak scaling experiments on Perlmutter
 - 160x64x64 Local Grid
 - Using Shell-D surrogate mechanism for gasoline (35 species)
 - 4 ranks/node (1 gpu/rank)
 - Scaled from 1 – 64 nodes

Baseline: Fortran S3D DBO Time/Iteration



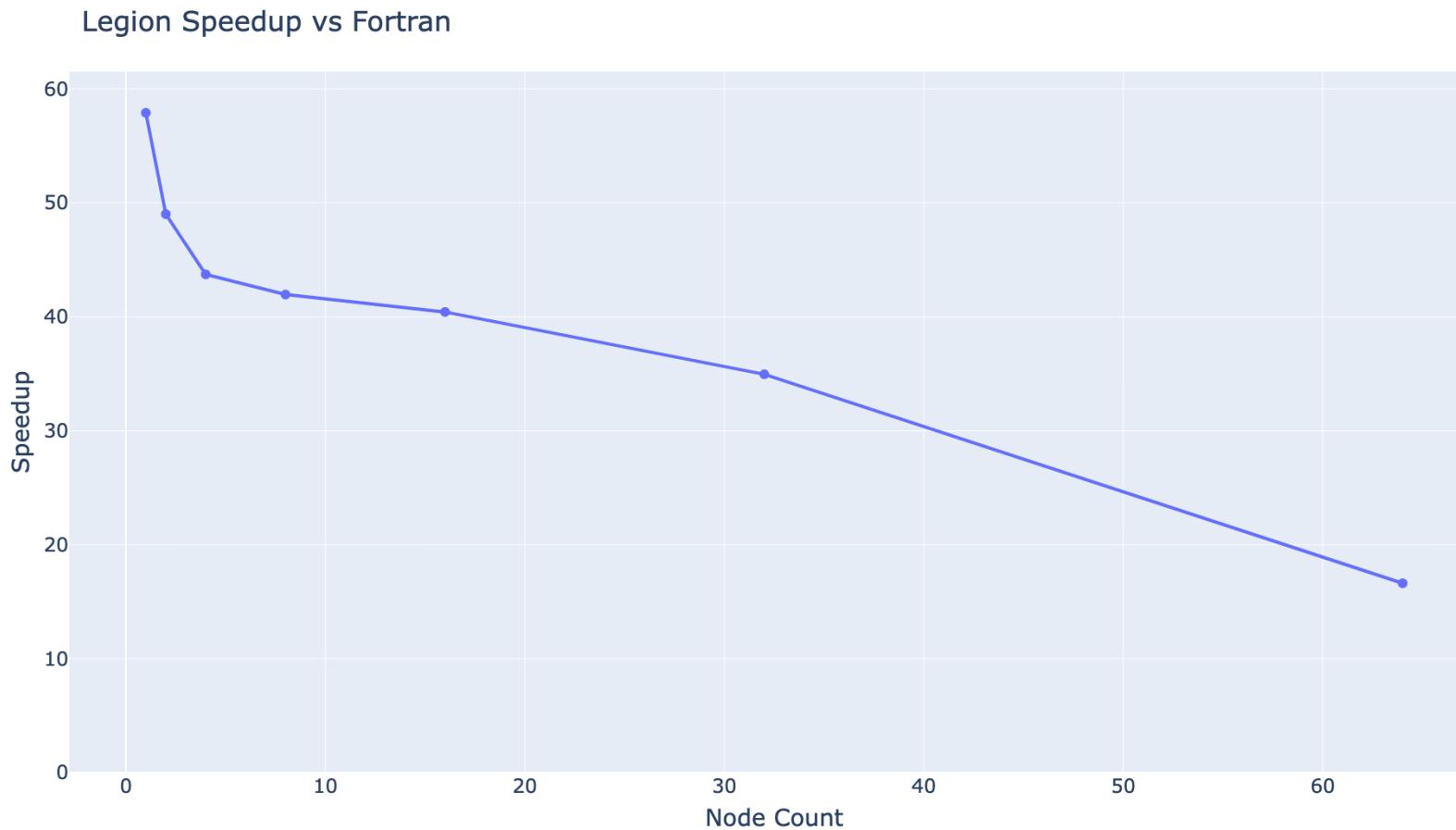
S3D Fortran takes ~40 to 45 seconds/timestep

S3D Legion/Regent DBO Time/Iteration



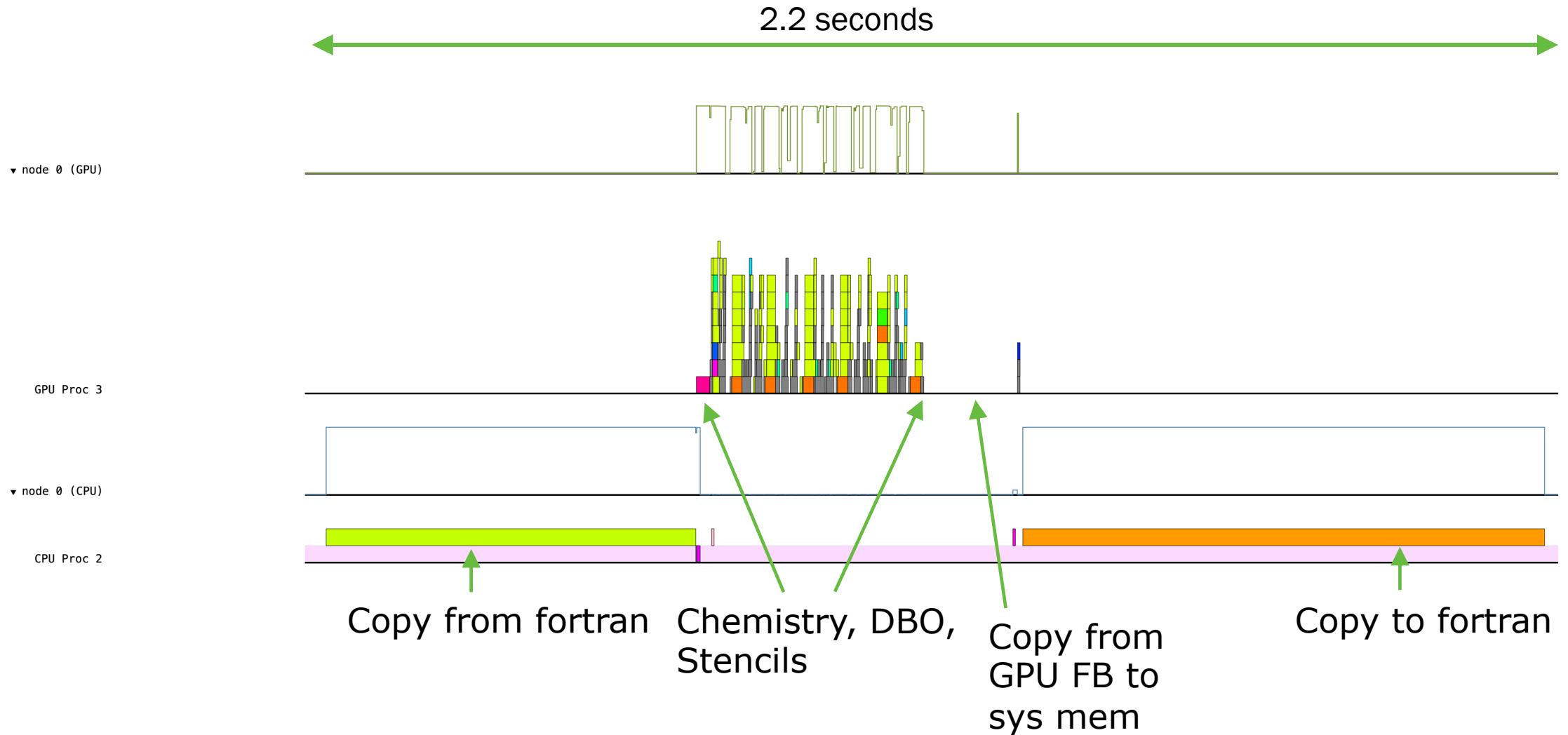
S3D Legion/Regent takes between 0.8 seconds to 2.7 seconds/timestep on Perlmutter, currently investigating slow down at 64 nodes

S3D Legion/Regent Speedup



Legion implementation is 16-60x faster than S3D-mpi implementation

Legion Prof Profile



In situ DBO ROM Timestep

Task	Percent of Timestep
copy_global	0.025
compute_funcF	0.478
compute_URHS	0.438
compute_funcZ	0.643
DBO_GETY	0.335
compute_inverse	1.530
reduce_global	0.008
compute_VRHS	0.040
IntegrateUmodesTask	0.276
IntegrateDBOTask	0.105
DBO_SPEC_RHS_IN_FUSED	0.977
DBO_SPEC_RHS_OUT_FUSED	0.405
TOTAL	5.261

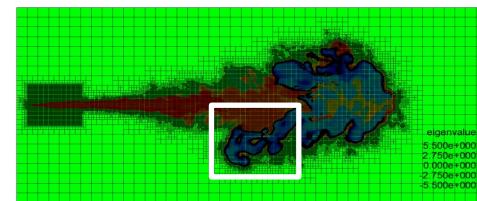
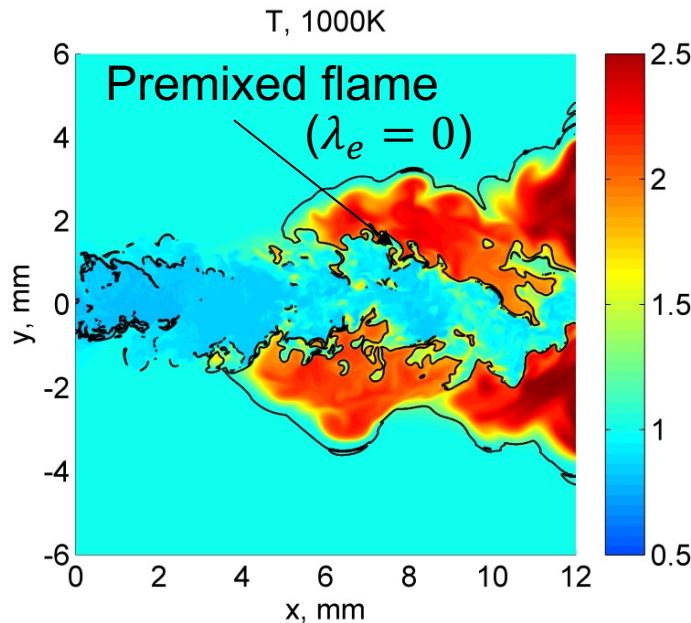
New DBO tasks take around 5% of total execution of timestep

Future work

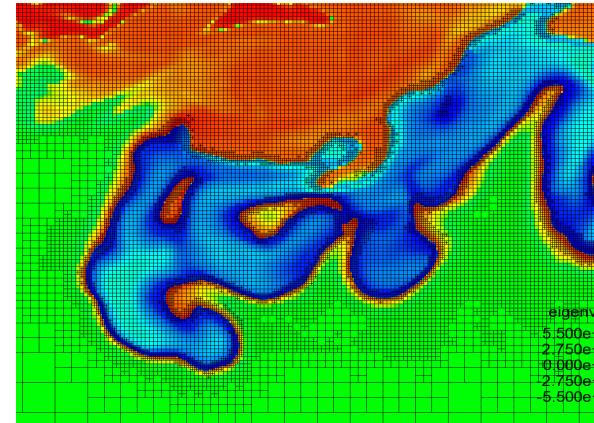
- Improve Legion weak-scaling performance on Perlmutter
- Move to rank/node configuration
 - Allow Legion runtime to manage 4 GPUs and use nv-link for intra-node copies
- DBO has been ported to Crusher/AMD GPUs, but currently crashes
- Scale S3D-DBO Legion/Regent on Summit, Perlmutter, Crusher and Frontier

In-Situ Chemical Explosive Mode Analytics (CEMA)

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

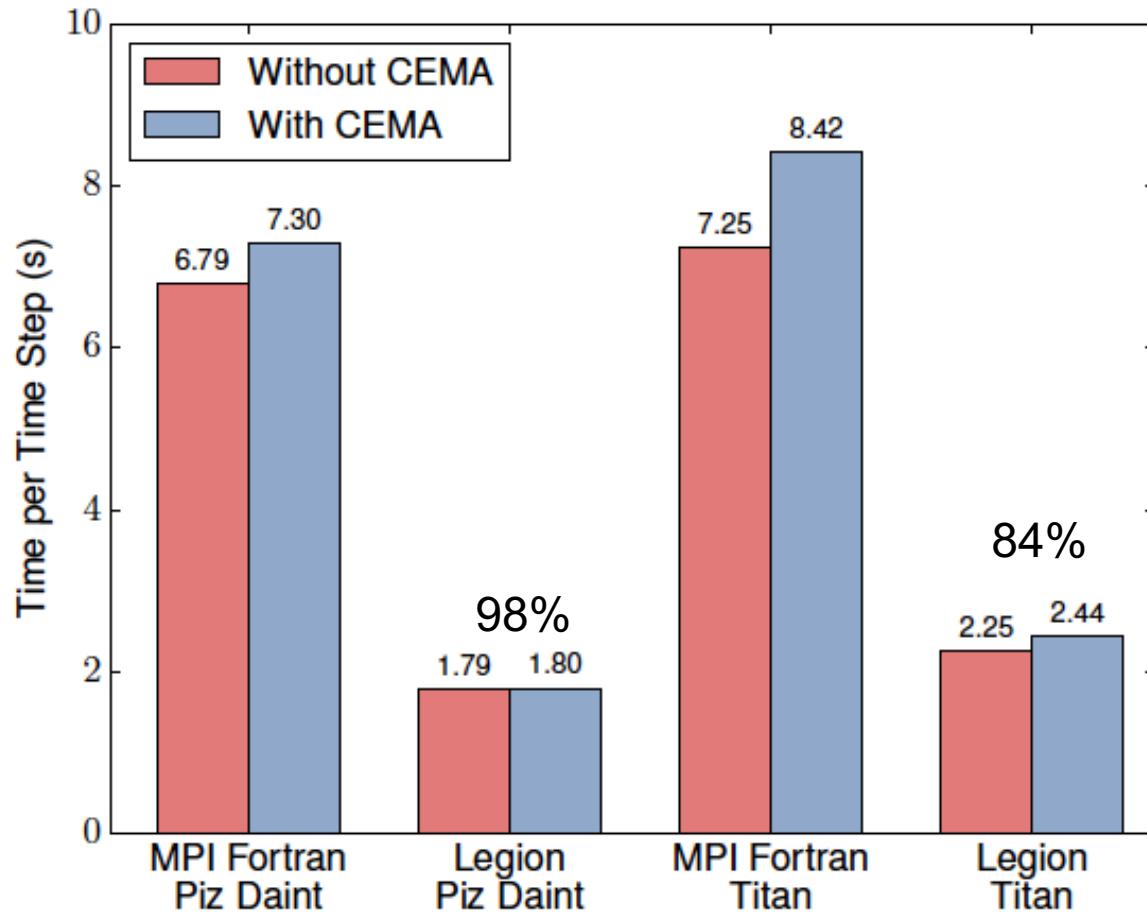


CEMA-based AMR
to capture premixed
fronts ($\lambda_e = 0$)



- 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)



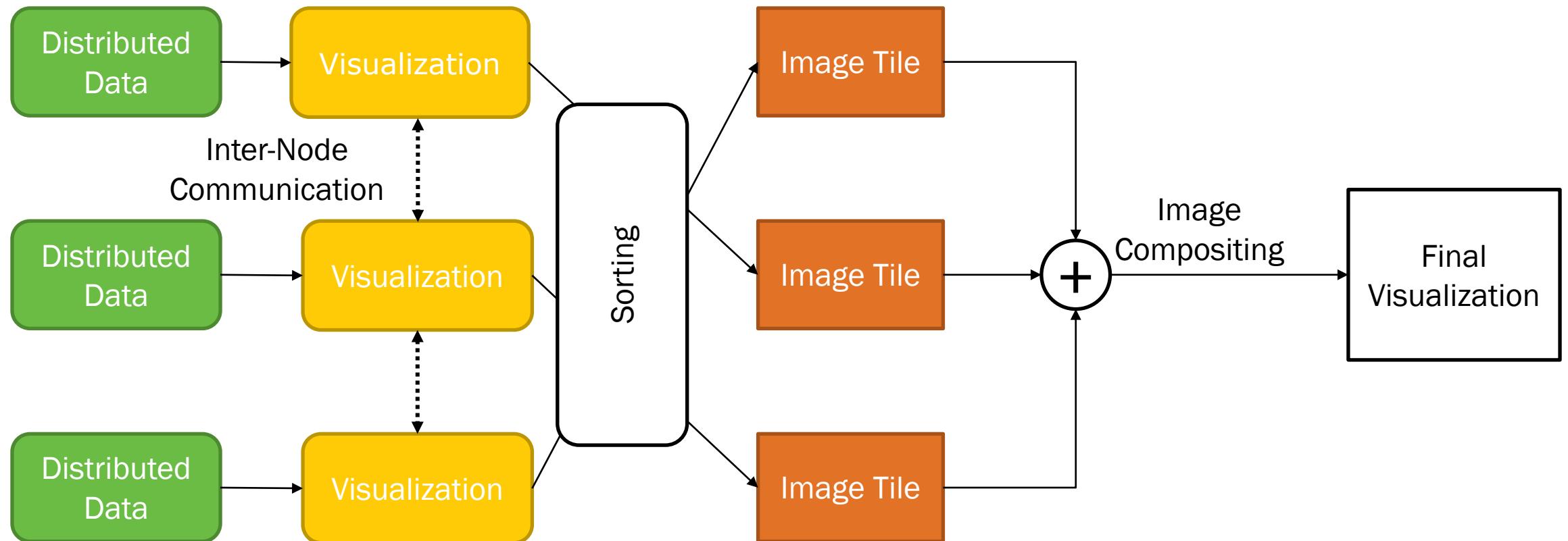
In situ Chemical Explosive Mode Analysis (CEMA) within the S3D Combustion Application – analysis results drive application parameters dynamically.

Reduced overhead of CEMA by a factor of 10 via adaptive/dynamic scheduling of analysis operations (**overhead now less than 2% of overall execution time**).

Runtime system analyzes and allows mapping of dynamic application workloads – e.g. infrequent, changing and data-dependent analysis and visualization operations.

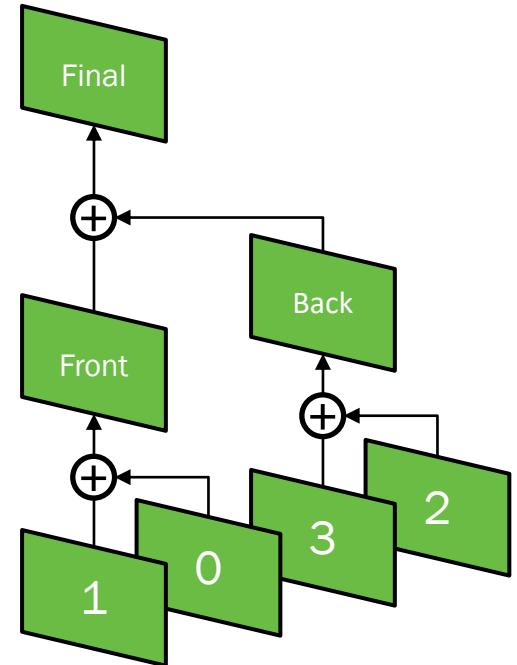
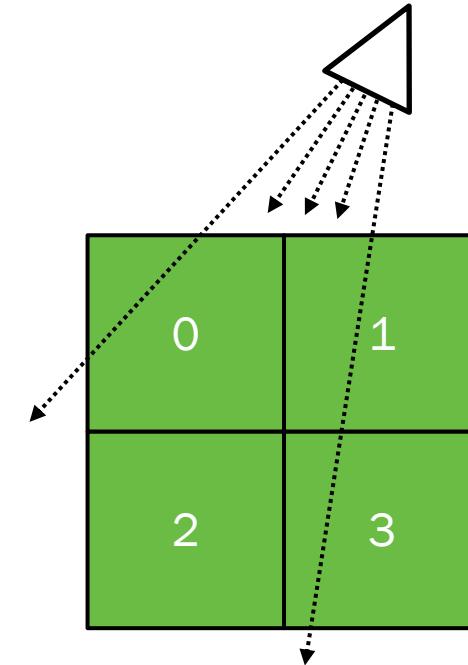
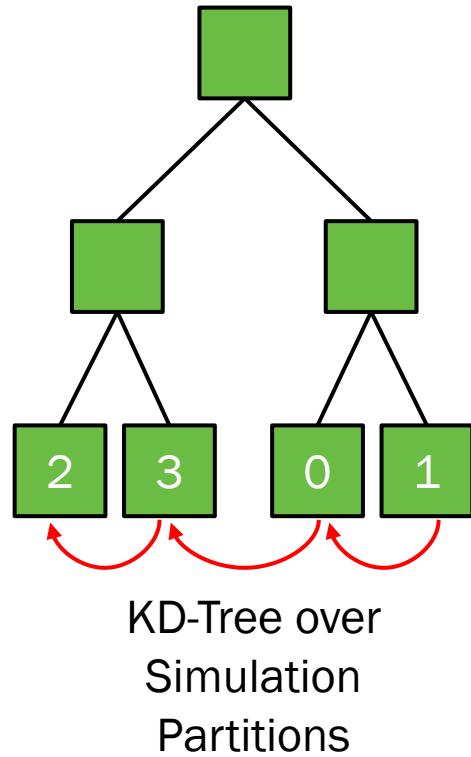
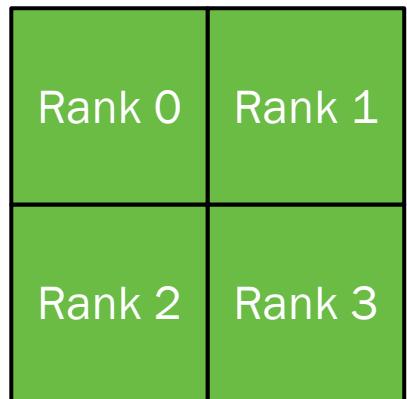
Coupling Visualization Pipeline with S3D MPI only

- Traditional Scientific Visualization Pipeline (Sort-Last)



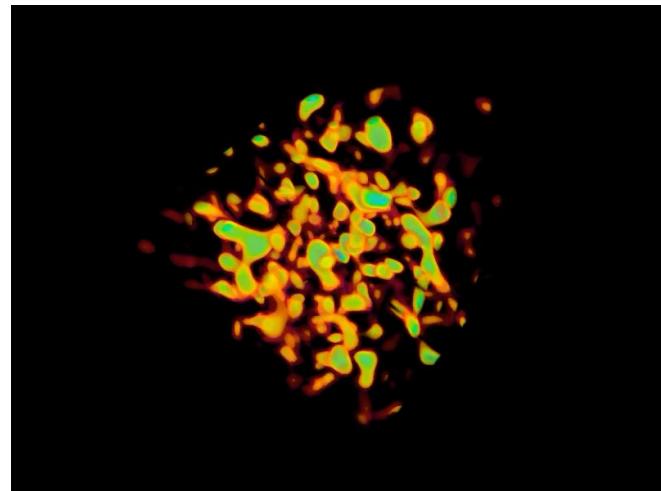
Coupling Visualization Pipeline with S3D Legion/Regent

- Sort-Last Image Compositing in Regent

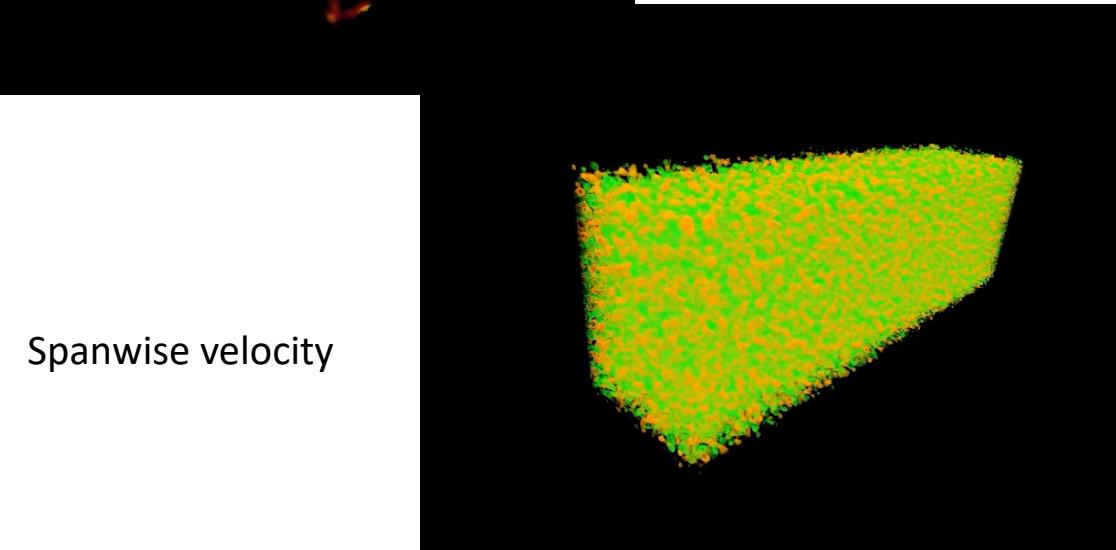


Coupling Visualization Pipeline with Legion/Regent

- Integration of Volume Rendering

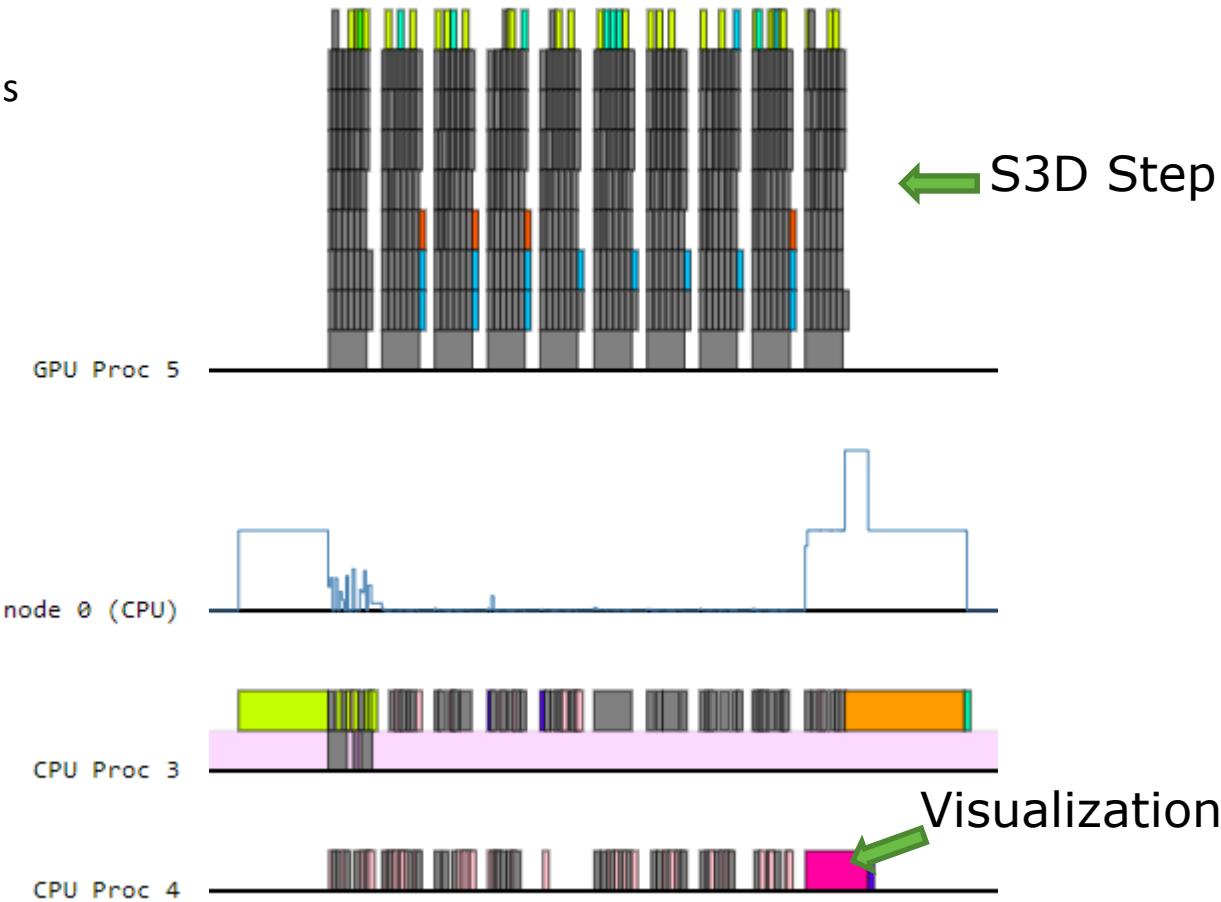


Temperature fluctuations



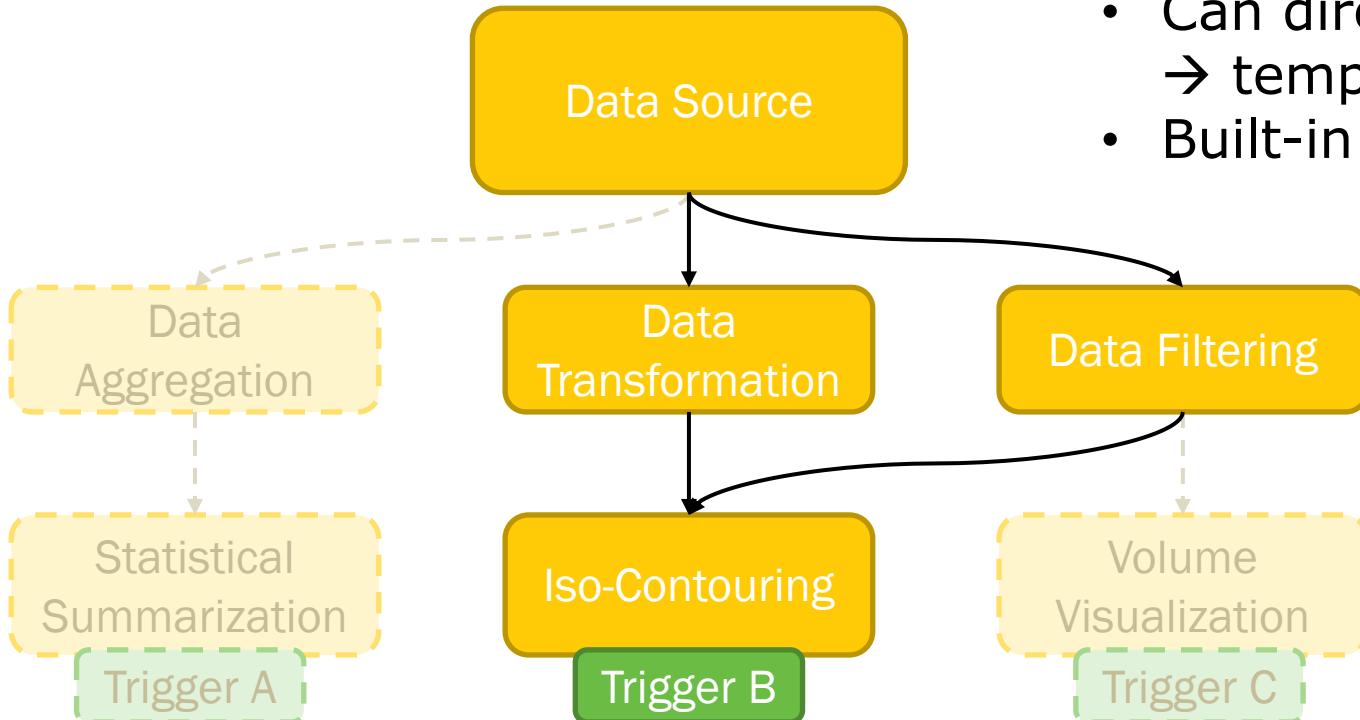
Spanwise velocity

Execute visualization every 10th step



Coupling Visualization Pipeline with Legion/Regent

- Adaptive In Situ Visualization
 - Construct Event-based Visualization Pipeline using Declarative and Reactive DSL
 - Easy to construct complicated triggers
 - Can directly filter time-varying variables
→ temporal logic
 - Built-in support for lazy evaluation



Declarative Specification

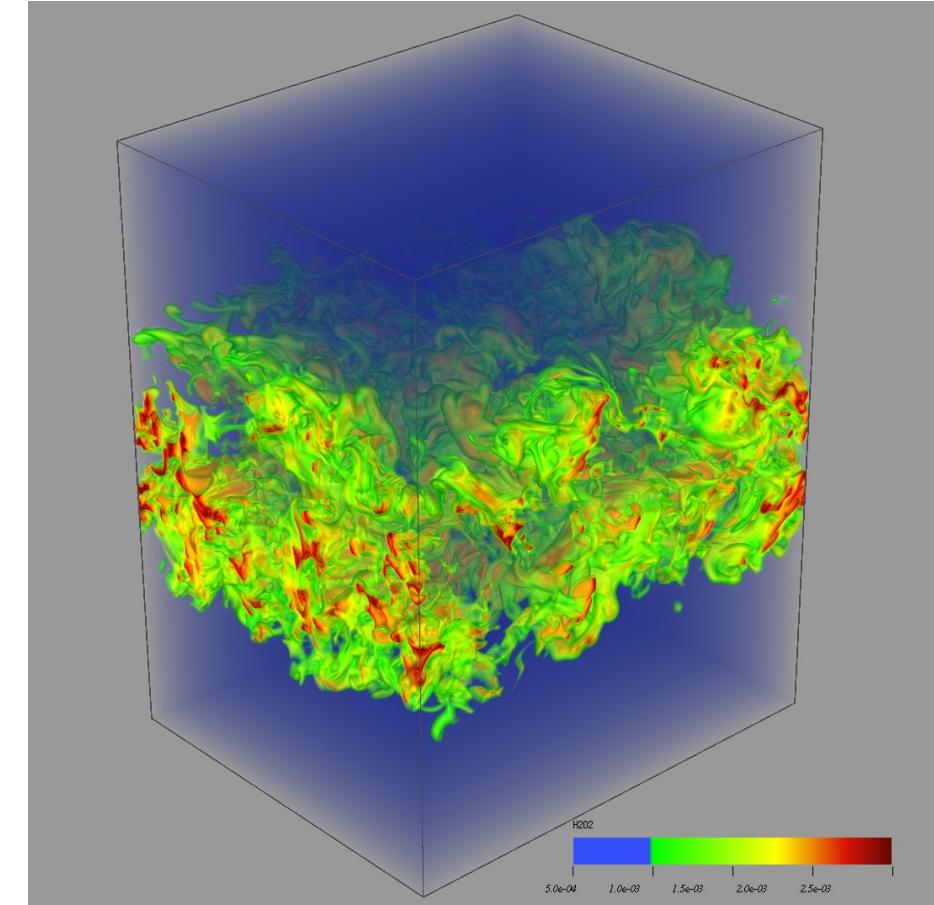
Compression Ignition anomaly detection / visualization using DIVA

Challenges:

- When and where an anomaly will happen is unknown
- Brute-force searching for anomalies at every timestep can be expensive
- Also need to study why anomaly happens (**causality analysis**)

Solutions:

- Multi-level triggers to reduce the computation cost (**DIVA directly supports triggers**)
- Memorize information near anomaly (**DIVA allows accessing historical values systematically**)



Declarative Specification

Compression ignition anomaly detection / visualization using DIVA

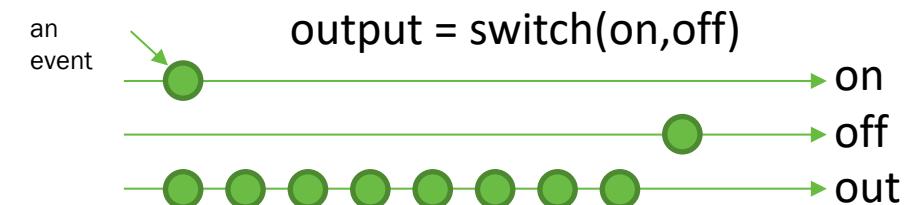
Declare pre- and post-anomaly events

```
anomaly      = valid && (m1 > 0.7 || m2 > 0.7)
pre_anomaly  = switch(on = valid, off = anomaly)
pst_anomaly  = countN(since = anomaly, n = 10)
```

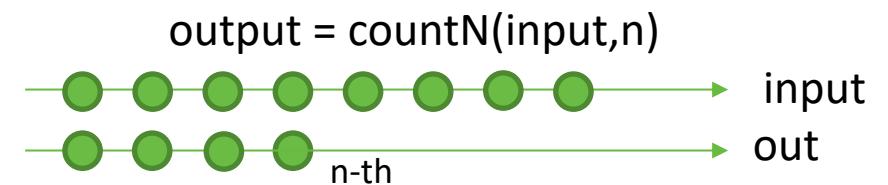


DIVA defines many built-in reactive operators:

1. Array Operator: sum, max, min, ...
2. Temporal Operator: first, until, next, **switch**, **countN**
3. Parallel Operator across decomposed domains: reduce
4. Other Special Operator: window



Continuously signaling events between a pair of on & off signals, simulating a light switch.



Signaling the first n events of input.

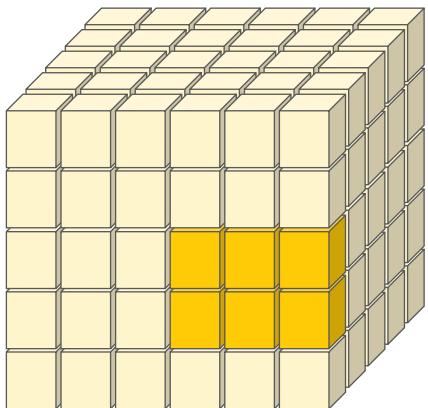
Declarative Specification

Compression ignition anomaly detection / visualization using DIVA

Declare statistical analysis

```
/* record pre-ignition statistics */
stats_ftr_avg = avg_list(features)
stats_ftr_min = min_list(features)
stats_ftr_max = max_list(features)
len = 40 /* record 40 steps */
recorded_avg = window(stats_ftr_avg, len)
recorded_min = window(stats_ftr_min, len)
recorded_max = window(stats_ftr_max, len)

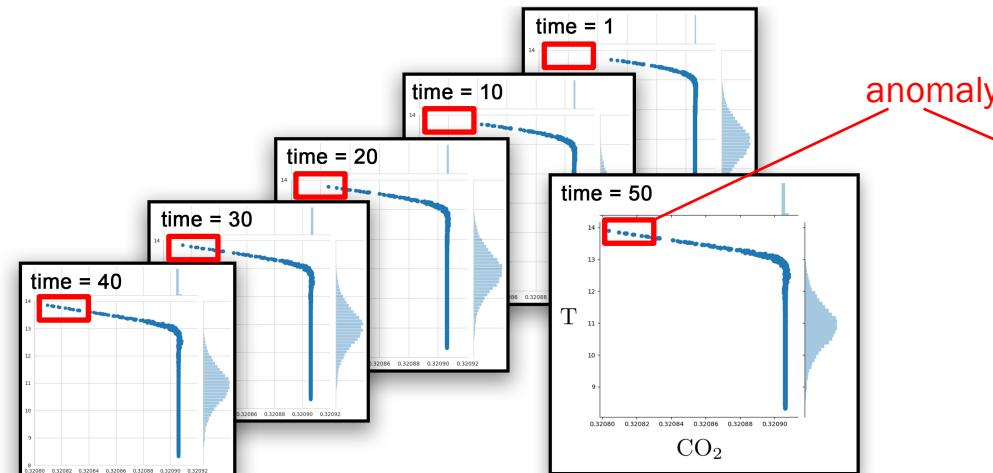
/* render the heat release after anomaly */
vol = volume(field = data.HeatRelease, /* ... */)
```



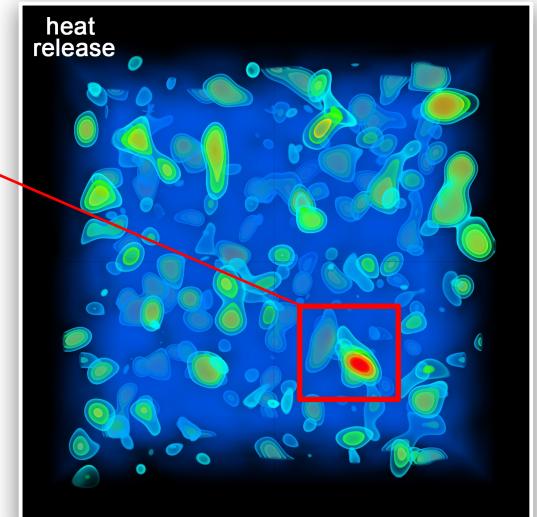
Select subdomains near anomaly

Conditions to trigger visualization

```
Trigger (valid) {
    print("m1=" + str(m1))
    print("m2=" + str(m2))
}
Trigger (anomaly) {
    save_statistics (data = recorded_avg, /* ... */)
    save_statistics (data = recorded_min, /* ... */)
    save_statistics (data = recorded_max, /* ... */)
}
Trigger (pst_anomaly) {
    save_ppm (vol, "img-" + str(time))
```



Visualize the statistics of sub-domains via joint-histograms
Using statistics collected prior to anomaly



Volume rendering after anomaly

Coupling Visualization Pipeline with Regent

- Integration of Adaptive In Situ Visualization Pipeline
 - Adaptive visualization generates highly dynamic workflows
 - Static task graphs lead to higher performance in Regent
- Method (work-in-progress):
 - Perform static code analysis
 - Split a visualization workflow into segments based on communication patterns
 - Generate a Regent task for each segment (reduce task launching overheads)
 - Use Regent to transfer data (avoid additional Regent-MPI handshakes)

Summary: Task-Based Systems Enable Complex Workflows at Extreme Scale

Goal: Future workflows will combine simulation, in situ ROMS, sensitivity analysis, uncertainty quantification, analytics and visualization at extreme scale -> need for productivity, composability, resilience, interoperability and scalability

Pros:

- Scientists write sequential code
 - Run in parallel
 - And distributed
 - And GPU
- No synchronization bugs
- Automatically asynchronous, automatic data movement
- Performance portability (mapper utility)

Cons:

- More explicit about data partitioning, tasks
 - For the system to help you, you need to tell it more about what you're doing

Questions: jhchen@sandia.gov

Acknowledgments:

DOE Basic Energy Sciences, Gas Phase Chemical Physics

DOE Office of Science Distinguished Sciences Fellows Award

ASCR Project on Collaborative: In Situ Visual Analytics Technologies for Extreme Scale Combustion Simulations

ASCR Exascale Computing Project

DOE INCITE, ALCC, and NERSC ERCAP Awards

SINTEF BIGH2 and AMAZE projects