Ignition of n-dodecane jets in a closed cylinder at 60bar,
computed with PeleLMeX on Frontier

Pele Combustion: Early Frontier Runs and Beyond

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NASA Ames, Moffett Field, CA

April 11, 2023

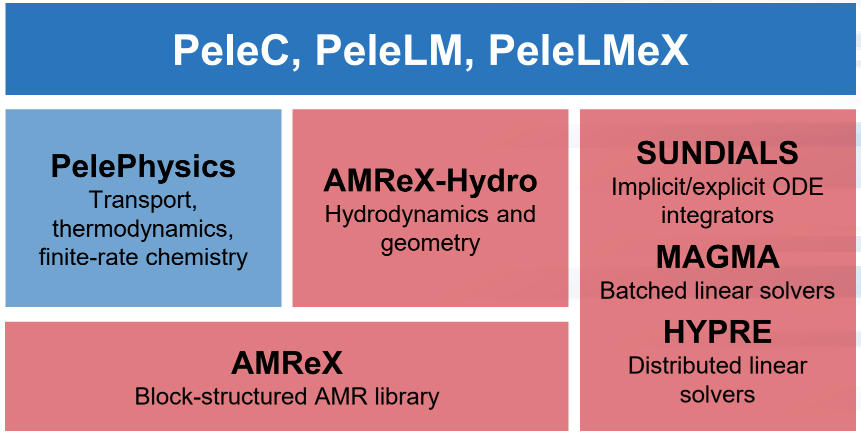
Overview of Presentation

- The Pele Suite of codes and analysis tools
- KPP2 Challenge and Demonstration Cases
- Porting details, performance
- Stretch goals and applications beyond our KPP

Pele Combustion Suite

Pele is the Exascale Computing Project's (ECP's) application suite for high-fidelity detailed simulations of turbulent combustion in open and confined domains

- Detailed physics and geometrical flexibility to evaluate design and operational characteristics of clean, efficient combustors for automotive, industrial, and aviation applications
- Targets simulation capabilities required to inform next-generation combustion technologies, for example:
  - Advanced internal combustion engines (e.g., RCCI)
  - Novel supercritical CO_2 power cycles
  - Rotating detonation engines
  - Supersonic cavity flame holders
  - Aviation combustors for sustainable drop-in JetA fuels



PeleC, PeleLM, PeleLMeX

PelePhysics
Transport, thermodynamics, finite-rate chemistry

AMReX-Hydro
Hydrodynamics and geometry

SUNDIALS
Implicit/explicit ODE integrators

MAGMA
Batched linear solvers

HYPRE
Distributed linear solvers

AMReX
Block-structured AMR library

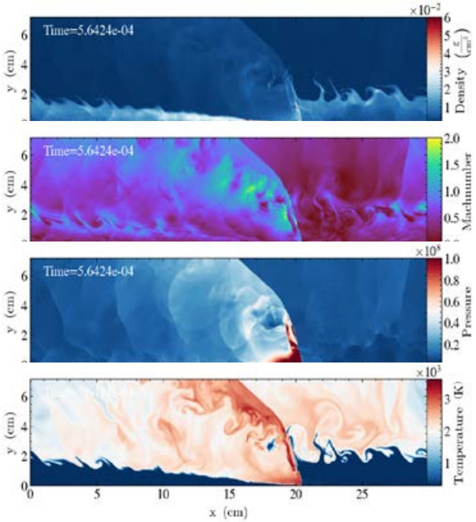
- Pele combustion simulation and analysis suite:
  - ***PeleC*** (compressible), ***PeleLMeX*** (low Mach) reacting flow codes
  - ***PelePhysics*** (thermodynamics, transport, chemistry models)
  - ***PeleAnalysis*** (in-situ, post-processing/analysis)
  - ***PeleMP*** [multi-physics] (soot, radiation, Lagrangian spray models)
  - ***PeleProduction*** (collaboration hub)

Open-source code developed under the Exascale Computing Project:
https://github.com/AMReX-Combustion

PeleC

Compressible flow solver

- Conservation of species mass densities, momentum, total energy
- Time-explicit Runge-Kutta (RK)-based advance
    - Time-explicit RK variants for diffusion and hyperbolics (PPM, PLM, WENO, MOL)
    - SUNDIALS-driven ODE integration for finite-rate chemical kinetics (CVODE, ARKODE)
- PelePhysics provides finite-rate chemistry models, equations of state and transport properties. Non-ideal thermo/chemistry modifications and tabulated lookup table models available
- PeleMP provides access to optional multiphase (spray) fuel models via AMReX particle capability
- https://github.com/AMReX-Combustion/PeleC



Rotating detonation engine
Sreejith NA et al., 2022

Compression ignition in a high-pressure combustion chamber, computed on Frontier as part of Exascale Computing Program Challenge Problem, 2023

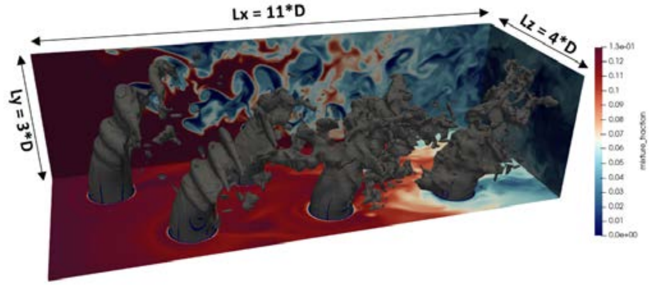
Supersonic cavity flame holder
Sitaraman et al., Combustion and Flame, 2021

PeleLM(eX)

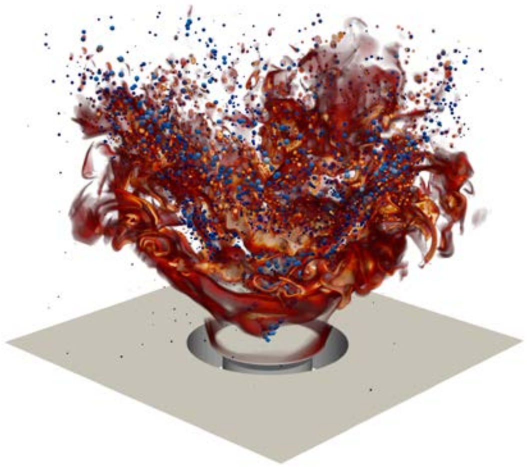
Low Mach flow solver

- Conservation of species mass densities, momentum, enthalpy
- Iterative/implicit variants of spectral deferred corrections time stepping for tightly coupled multi-physics systems – required for **large dt** enabled by the low Mach algorithm
  - Semi-implicit (Crank-Nicolson) diffusion, Godunov-based advection
  - SUNDIALS-driven ODE integration for finite-rate chemical kinetics (CVODE)
- PelePhysics provides finite-rate chemistry models, equations of state and transport properties. Tabulated lookup table and neural-net-based models available for turbulence/chemistty models
- PeleMP provides access to optional multiphase (spray) fuel models (Lagrangian, AMReX particles based), moment-based soot models, and radiation transport
- Critically, the low Mach model requires the solution of a linear elliptic system to compute the constrained spatially isobaric solution, and a set of linear systems for the implicit diffusion solve. *Due to geometry-induced ill-conditioning, the elliptic systems often require HYPRE's BoomerAMG, with robustified, iterative smoothers*
- ***PeleLMeX's non-subcycled integrator supports AMR with closed-chamber pressurization due to fueling and heat release***

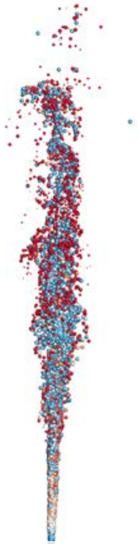
https://github.com/AMReX-Combustion/PeleLM
https://github.com/AMReX-Combustion/PeleLMeX



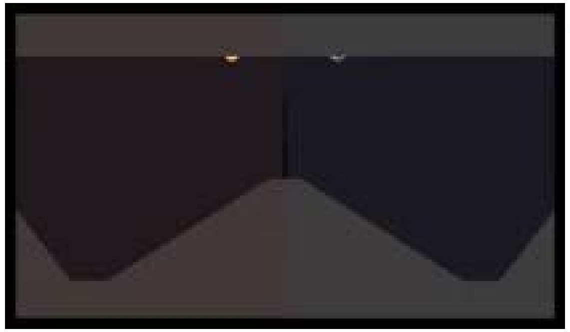
Gas turbine premixer, PeleLM
M. Vabre, B. Savard, et al.,
CICS Spring Technical Meeting, 2022



Aero-engine spray flame stabilization with SAF fuel (C1-ATJ), B Soriano, et al



Lagrangian fuel sprays in PeleLMeX
(droplets colored by Temp)
Ariente et al., in prep, 2022

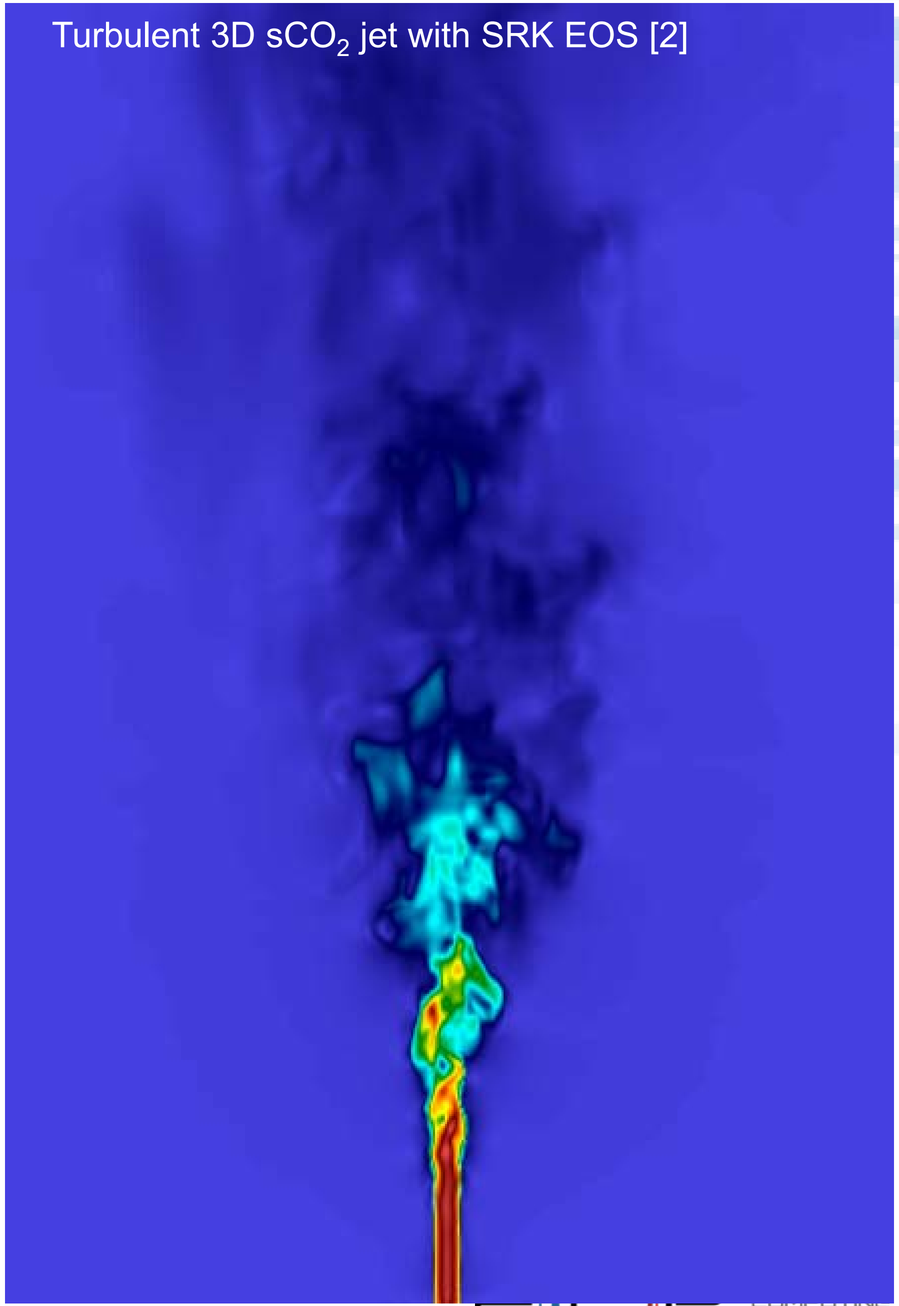


Quad n-dodecane jets into KPP PB
Wimer, Esclapez, et al., in prep, 2022

PelePhysics

An open-source combustion physics library

- https://github.com/AMReX-Combustion/PelePhysics
- EOS: ideal gas mixtures (CHEMKIN), Soave-Redlich-Kwong (SRK), EOS lookup tables / neural nets
- Models and parameters for thermodynamics
- Mixture-averaged and unity Le transport properties, including extensions for non-ideal gases
- Chemical reactions and finite-rate chemistry integration via SUNDIALS
- Python-based C++ generator to convert CHEMKIN combustion models into production rate and reaction Jacobian code for CPU/GPU evaluation, including optional quasi-steady-state assumptions (QSSA) for automated model reduction



Turbulent 3D sCO_2 jet with SRK EOS [2]

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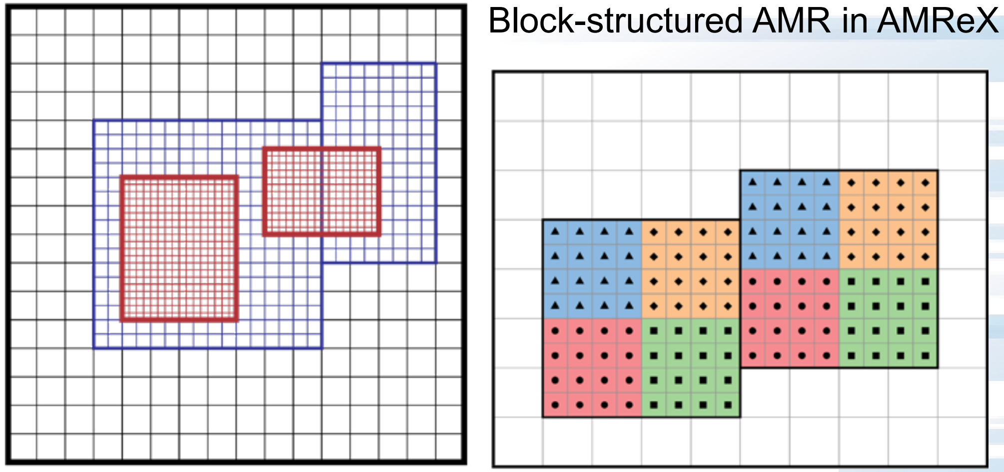
[2] Ream et al., SIAM CSE, 2021

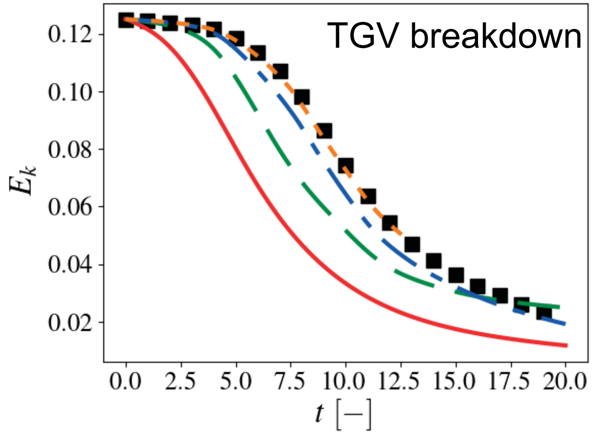
Pele Methods and Tools

All Pele tools exploit block-structured AMR

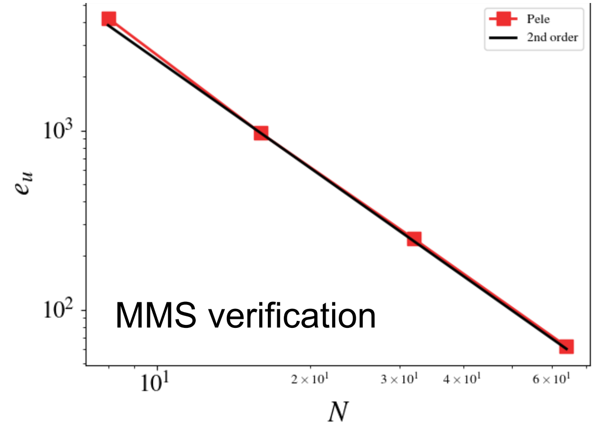
- We extensively leverage AMReX library (data structures, communication, parallelism, GPU acceleration, …)
- Conservative cross-refinement finite-volume methods
  - PeleC: Time-explicit RK variants for diffusion and hyperbolics (PPM, PLM, WENO, MOL) with temporally split chemistry evolution
  - PeleLM(eX): Iterative/implicit SDC-variants for tightly coupled ADR systems resulting from large dt via the low Mach algorithm
- PeleC: Subcycling supports constant CFL time advance strategy across AMR hierarchy. PeleLMeX utilizes a non-subcycled time advance to support AMR with closed/pressurizing chambers
- Pele's CI supports formal design order verification through method of manufactured solutions (leveraging MASA library)
- AMR-aware in situ and post-processing tools (surface, slice and stream tubes/line extraction, high-dimensional sampling/statistics, CEMA and reaction path analysis, ROM/ML training, table/NN physics lookup, subsetting, demand-driven processing IO, etc.)



Block-structured AMR in AMReX



TGV breakdown



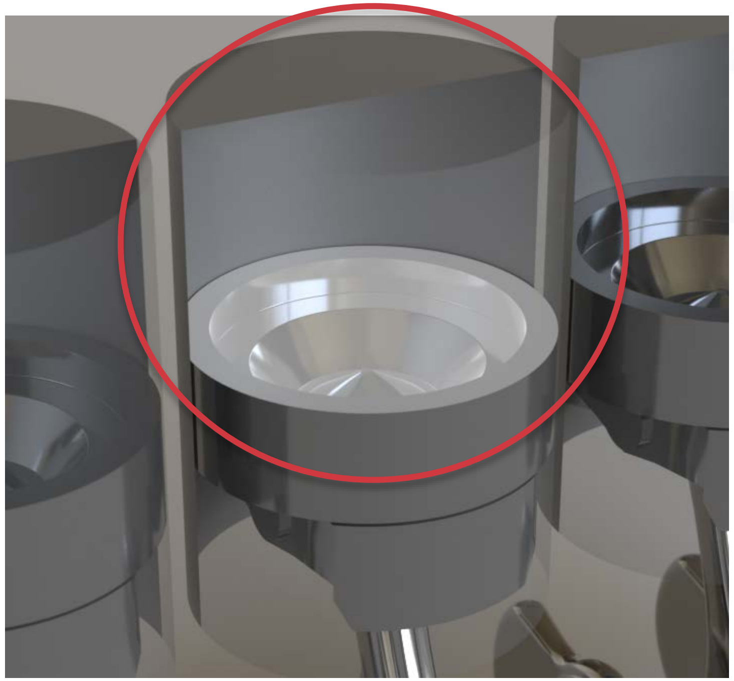
MMS verification

Combustion-PELE KPP2 Challenge Problem

Dual pulse injection of combustion fuels w/varying reactivity into engine-relevant geometry

- Baseline enabling simulations to isolate effects of spray evaporation on mixture composition and temperature, use of alternative fuels, and combustion phasing control
- Scoped to consume 2-4 weeks on a significant fraction (~75%) of Frontier's resources

- **Geometry:** Domain relevant to engine cylinder (see figure)
  2.5 cm, flat cylinder head, shaped piston surface
- **Fuel:** *n*-dodecane/methane QSS model (35 species)
  Initial chamber gas: ϕ=0.4 CH_4 turbulent mixture, at 60 atm, 900K
  Jets: Re=14k, mixture *n*-dodecane(45%):chamber-gas(55%)
- **Strategy:** 4 symmetric jets, dual pulse, gas-phase injection
- **Resolution:** 0.85 μm cells (due to 60 atm environment)
- **Sim. Time:** 1 msec (based on jet transit, ignition delay)
- **Flow solver:** PeleC (AMReX-based compressible reacting flow)
- **AMR:** **6 levels** of factor-of-2 refinement
  Level 0-6: volume = (100,23,8.5,1.7,1.1,0.76,0.56)%
  Cell count/level = (0.03,0.06,0.8,0.3,1.5,8.4,49.5) B
  Total cell count ~ 60B (2.4T dofs)



Measure of Capability to Perform Challenge Problem

Goal:

- Complete 30-60 min run with PeleC (compressible code) using 75% of available Frontier resources
- Allows confident extrapolation of ability to simulate the full challenge problem

Strategy/setup:

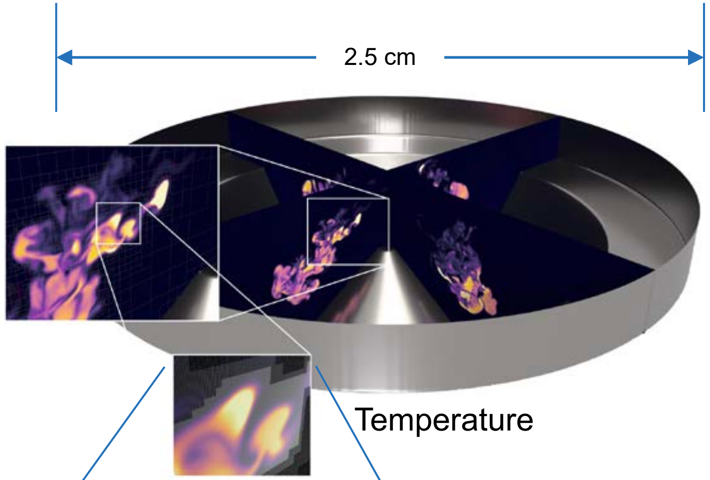
- Begin with a pre-evolved lower-resolution simulation of the same physical configuration to ensure sufficiently developed flow fields: jet mixing and penetration into domain, combustion ignition, etc.
- Restart with 3 additional factor-of-two refinement levels to reach full problem specification

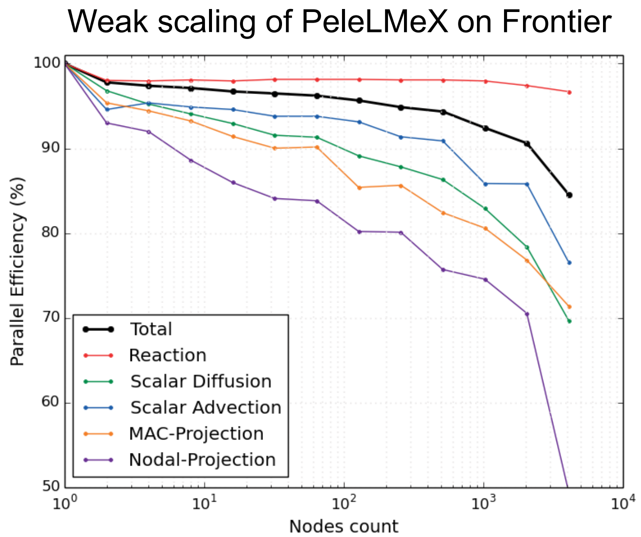
Expectations:

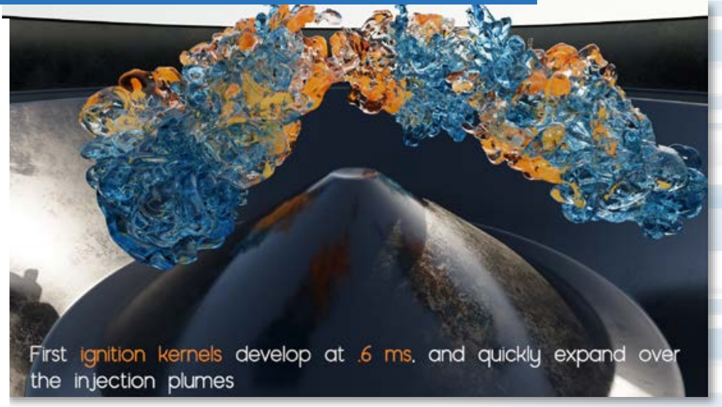
- A recent *n*-dodecane flame (1/300 scale) computed with ***PeleLM***, required 230 sec for a 5 μs coarse-grid time step on 6000 Theta KNL cores. On 75% of Frontier, based on peak flops, we expect a reduction of 14.8X, or 15.5 sec time step, that is 5 ms simulated time / month
- Assuming 50% weak scaling efficiency loss, and a 10X reduction in CFL time step due to use of compressible (PeleC) vs. low Mach (PeleLM) model
- Estimated Frontier wall-clock resources: 0.2 ms/month (30 minutes to evolve solution 0.19 μs)

Achieved Performance: 0.12 μs physical time in 41 min wall-clock, using 7k Frontier nodes (2.2X slower than estimates)

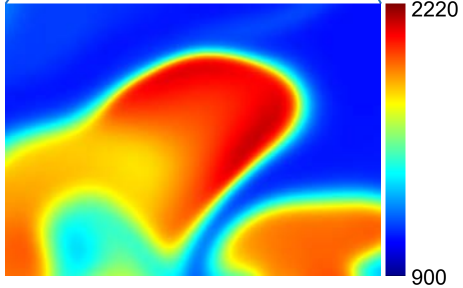
Combustion-PELE KPP2 Challenge Run



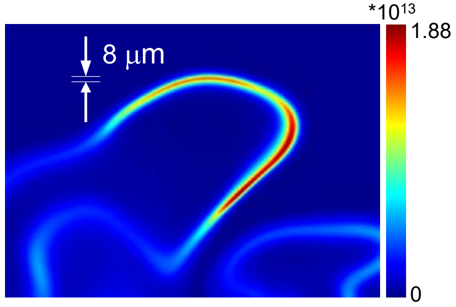

Weak scaling of PeleLMeX on Frontier



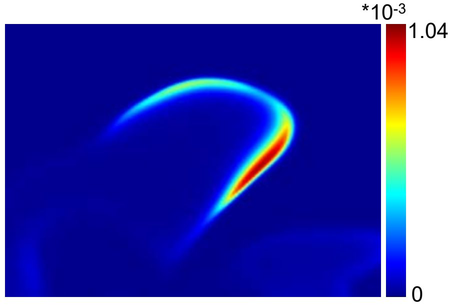
Precursor solution, showing jet-induced vorticity (blue) and ignition kernels (orange)



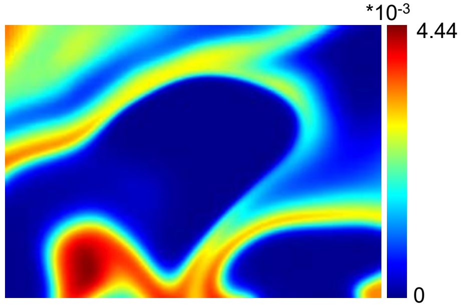
Temperature (K)



Heat Release (erg/cm^{3}s)



Y-OH



Y-CH2O

7-Level AMR PeleC simulation

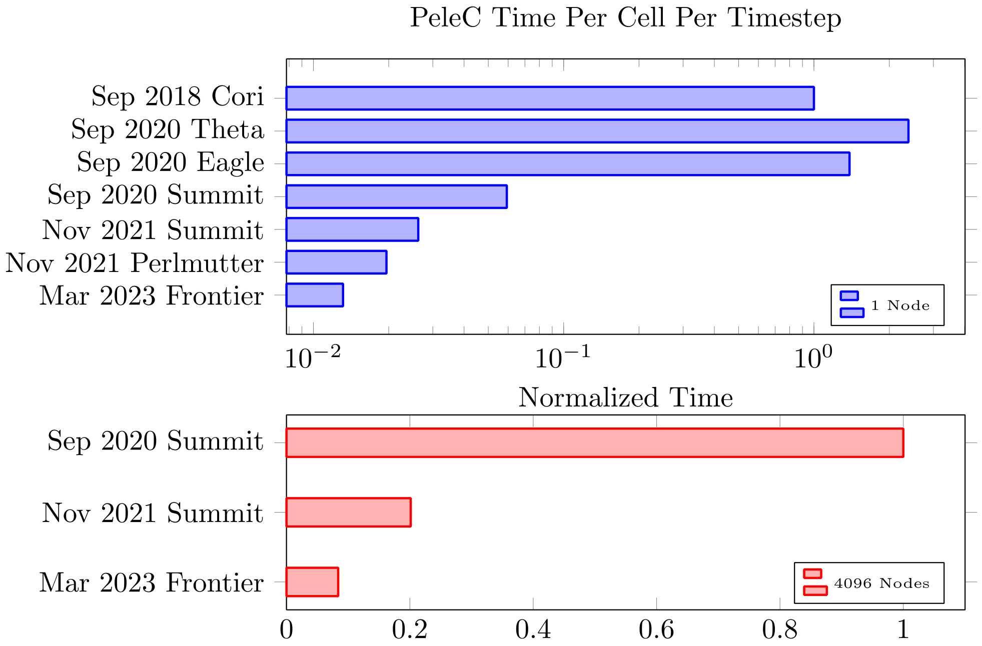
- Initial domain: 60atm, 900K, ϕ=0.4 CH_4 turbulent mixture
- Effective resolution: $(32{,}768)^2$ x 8192 with 0.6% of the domain at dx_{Fine} = 0.85 μm
- Four Re=14,000 fuel jets (45% n-dodecane, 55% initial chamber gas)

Notes:

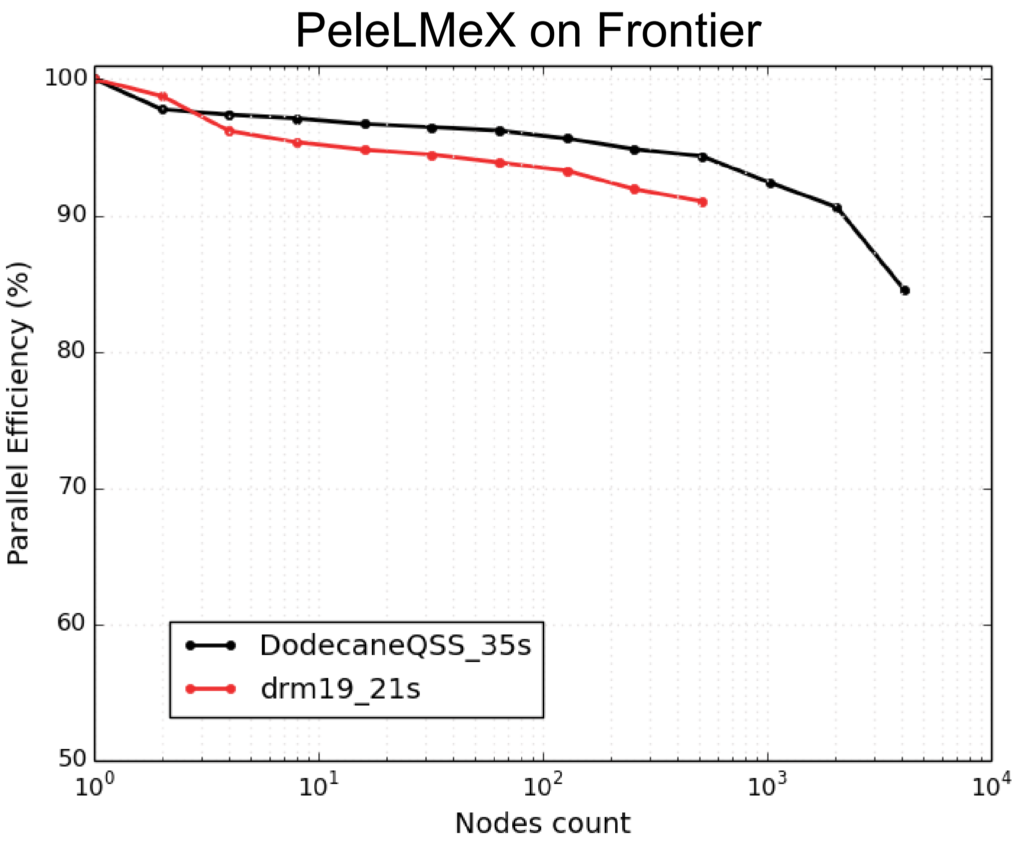
1. Weak scaling data for PeleC not yet available
2. Chemistry component scales nearly perfectly (same for both codes)
3. Communication-heavy operations scale poorly at high node counts – we expect similar issues with PeleC:
    - Load imbalance
    - Network-dependent

Running on Frontier - User experience

- PeleC: 75X performance gains over the last 4-5 years
- Stretch goals: PeleLMeX scaling on simpler problem:
  - Decent scaling results, 83% on 4096 nodes



PeleC time per cell per timestep from September 2020 code using `drm19` 21 species mechanism on Theta, Eagle, and Summit compared to November 2021 and March 2023 code using `dodecane_lu` 53 species mechanism on Summit, Perlmutter, and Frontier. 21 species case linearly scaled to approximate a 53 species run time.



Porting Pele codes to Frontier

Pele is a KPP2 project – Original software developed entirely under ECP

- First version of PeleC developed from CASTRO, a compressible Astro code
  - Mixed Fortran/C++ implementation, traditional for BoxLib/AMReX applications
  - Targeted many-core KNL architectures using MPI plus OMP offloading
- GPU ports
  - Initial PeleC was based on OpenACC, while preserving original Fortran/C++ structure
  - Simultaneously, AMReX developed a Kokkos-like portability layer
    - Pele codes were refactored to remove Fortran and use new AMReX layer
    - Initially used unified virtual memory (UVM) to simplify port, but UVM ultimately removed for performance on Frontier
    - Both implementations (CUDA, OpenACC) showed comparable performance
- Largest performance gains in Pele were via SUNDIALS chemistry implementation
  - Explicit RK-based solver replaced with implicit integrators, including CVODE+MAGMA

Performance Tuning of Pele

At the Pele level

- CEPTR, Pele’s Python-based code generator for complex chemistry/thermos
  - Supports quasi-steady approximations (production=destruction), algebraic rather an ODE, expressions for evolution of minor species, considerably more complex and memory intensive Jacobian evaluations
  - Heavily refactored chemistry and thermo expressions to minimize thread private arrays and pre-compute, unroll complex evaluation code with user-controlled levels of subexpression reuse
- Expanded use of SUNDIALS interfaces to MAGMA, CVODE

At the AMReX level:

- Fused kernel launches allowed higher device throughput when using smaller AMR boxes
- Implementation of asynchronous ghost cell exchange

Pele Stretch Goals

- Low Mach Pele
- Turbulence and turbulence chemistry models
- Multiphase (spray) fueling
- Radiation
- Soot

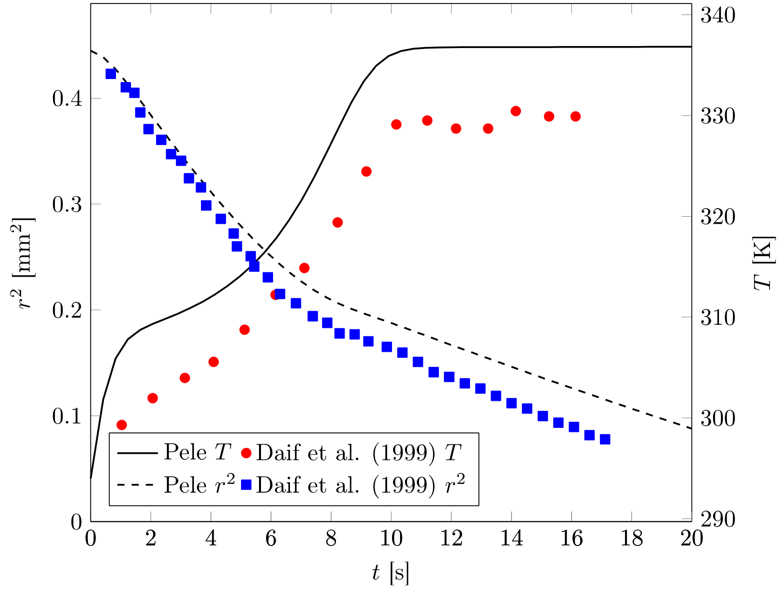
PeleMP: Overview

- Couples with the PeleC and PeleLMeX flow solvers
- Lagrangian dilute spray model
- Eulerian hybrid method of moments soot model
- Radiation: P1 gray gas model and the Planck-mean spectral model for the gas products and soot
- Hosted on GitHub as part of the AMReX-Combustion project
    - Github.com/AMReX-Combustion/PeleMP
- Documentation through GitHub Pages
- Pele flow solvers contain continuous integration for soot and spray functionality and coupling

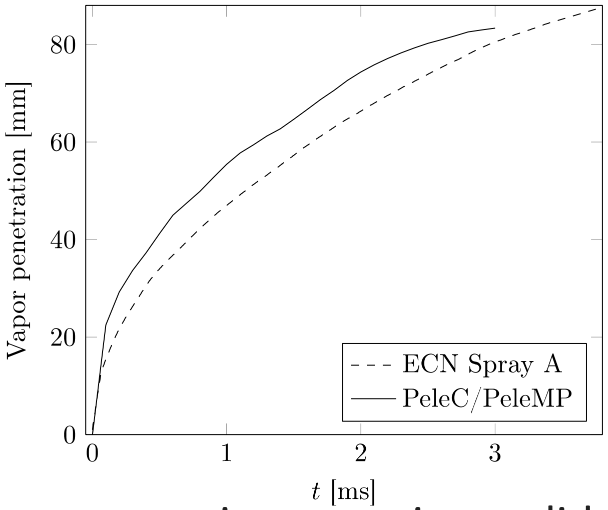
PeleMP: Spray Modeling

- Assume droplets are spherically symmetric and spatially uniform
- Two-way coupled with Eulerian gas-phase
- Multicomponent liquid evaporation model
  - From Tonini, S. (2006), Doctoral Thesis
- Proper particle handling with AMR and EB
- Templated injection routines with droplet diameter distributions
- Verification and validation using single droplet and spray injection cases
- Weak scaling test: uniformly distributed convecting particles

Daif, A., et al. *Journal of thermophysics and heat transfer* 13.4 (1999): 553-555.



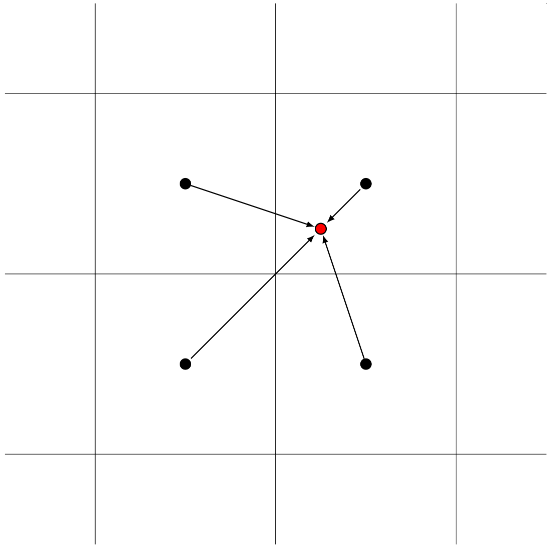
Multi-component single droplet evaporation validated against experiment

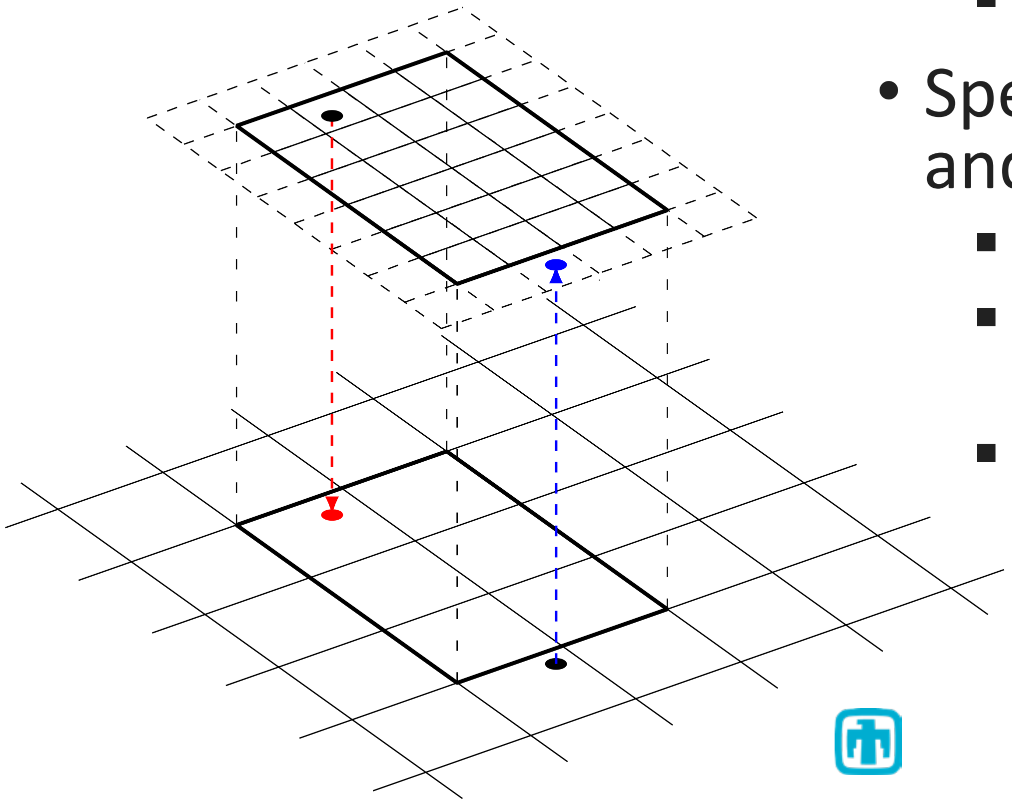


Vapor penetration over time validated against ECN Spray A

Pickett, L. and Abraham, J. P. *Atomization and sprays* 20.3 (2010): 241-250. Issn 1044-5110

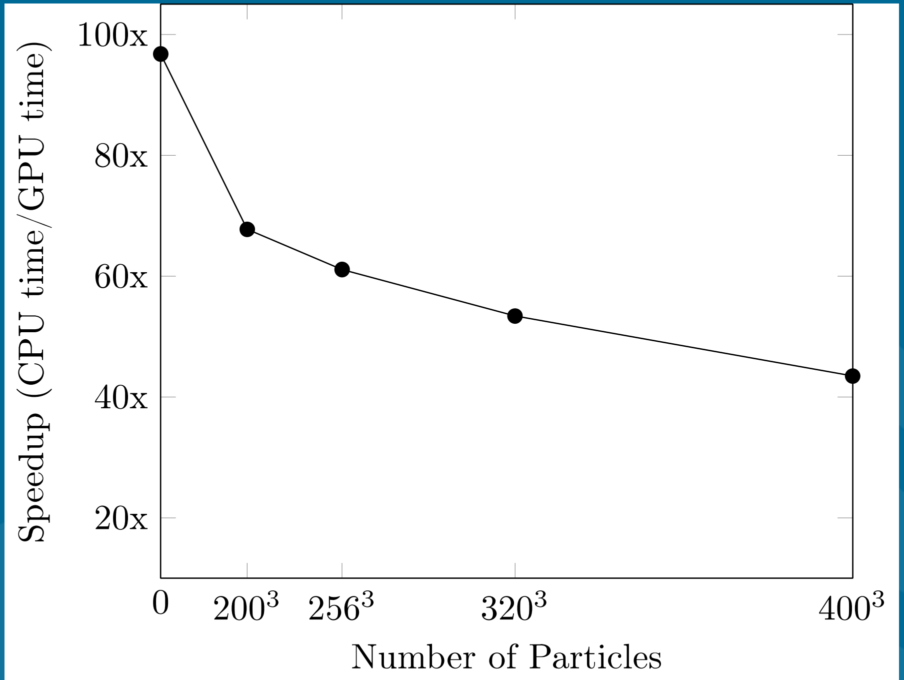
Lagrangian-Eulerian Coupling





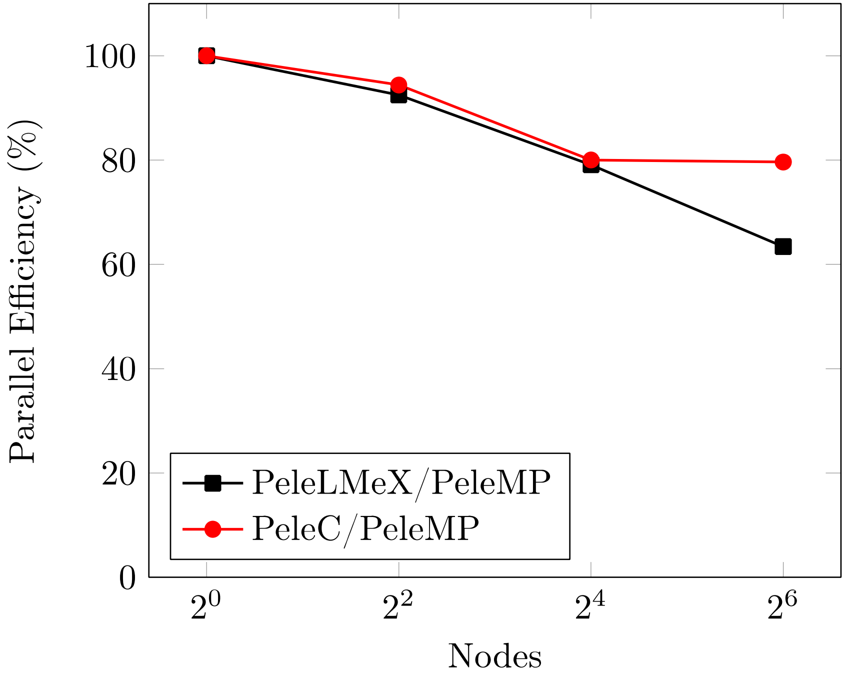
- Two-way coupled with gas-phase
  - Interpolate gas phase state to parcel location
  - Distribute sources to nearest cell center
  - Mass, momentum, and energy source terms
- Special care when interacting with box patches and AMR
  - Virtual and ghost particles
  - Virtual particles: finer mesh particles copied to coarser mesh (red dot)
  - Ghost particles: coarser mesh particles adjacent to finer mesh boundary (blue dot)

Performance of PeleMP sprays coupled with Pele



Comparing speedup between 8 nodes on Cori Haswell (CPU only) and 8 nodes on Summit (CPU/GPU)

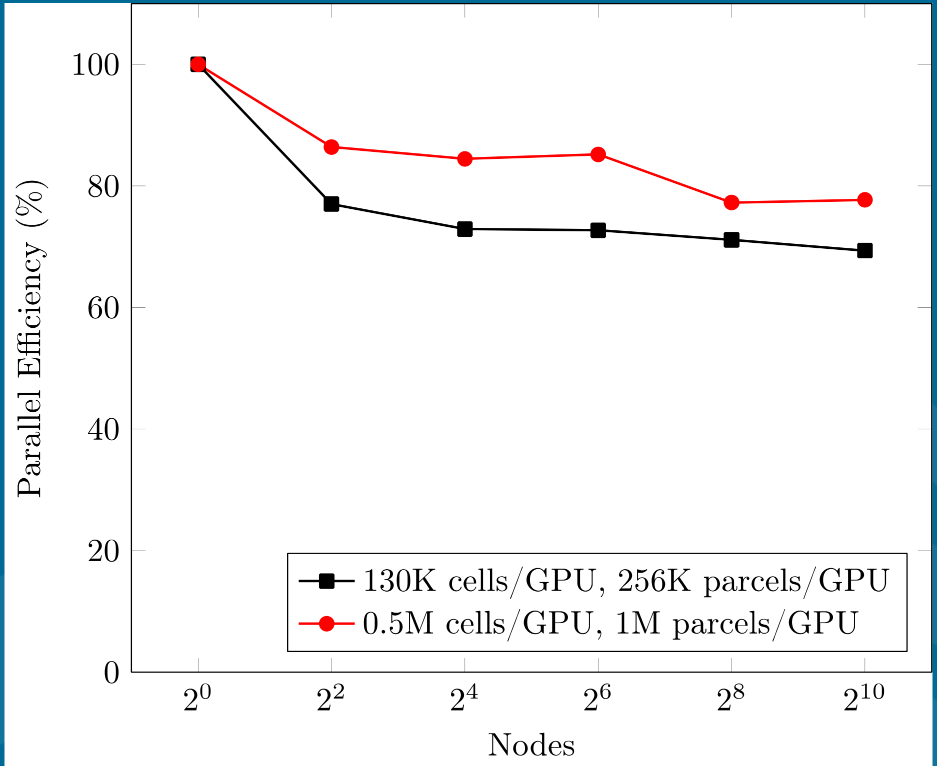
Summit has 6 NVIDIA V100 GPUs per node



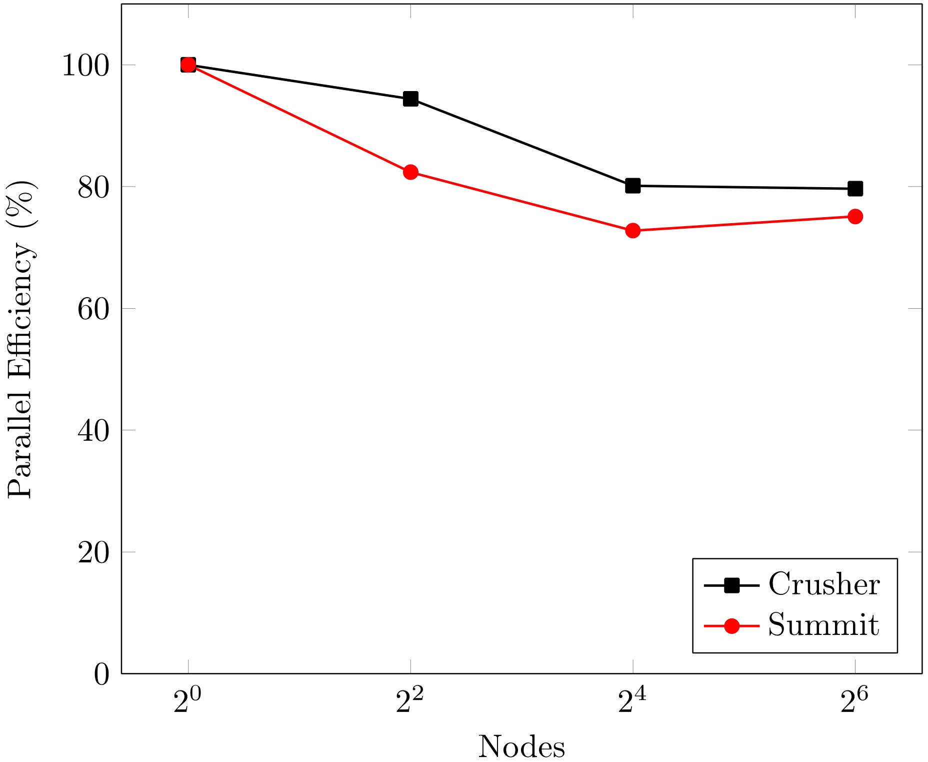
Weak scaling of PeleMP coupled with PeleC and PeleLMeX on Crusher; 262K cells/GPU and 512K parcels/GPU

Crusher has 4 AMD MI250X per node with 2 graphic compute dies each

Performance of PeleMP sprays coupled with PeleC and PeleLMeX



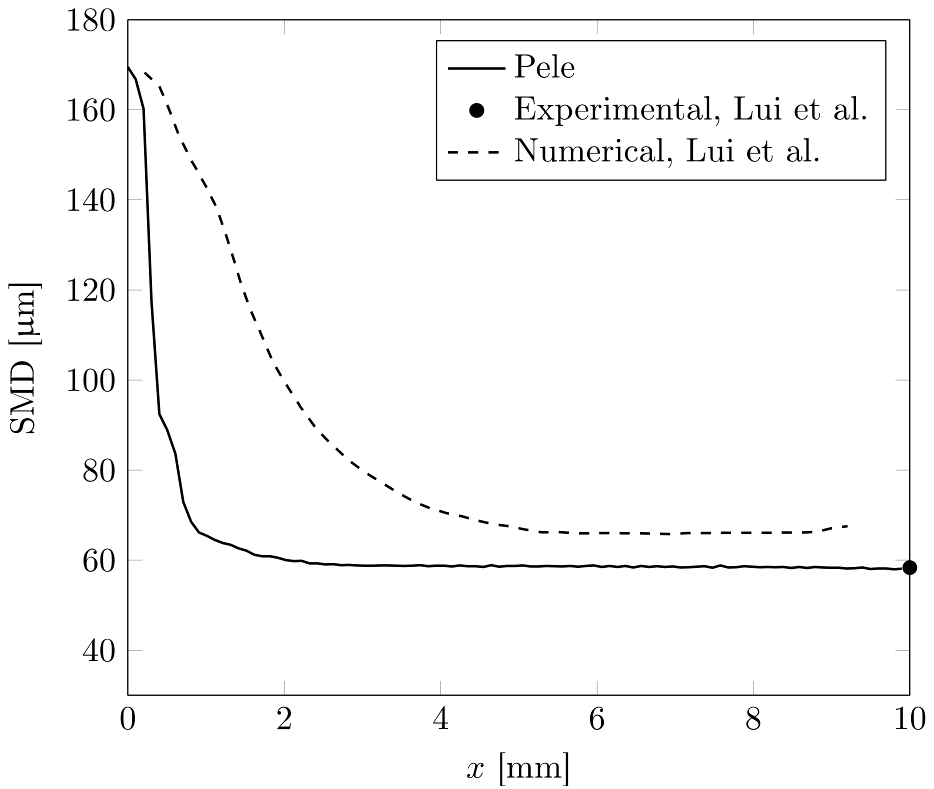
Weak scaling of PeleC/PeleMP on Perlmutter



Weak scaling of PeleC/PeleMP on Crusher and Summit; 262K cells/GPU and 512K parcels/GPU

Perlmutter has 4 NVIDIA A100 GPUs per node

Upcoming Spray Capabilities

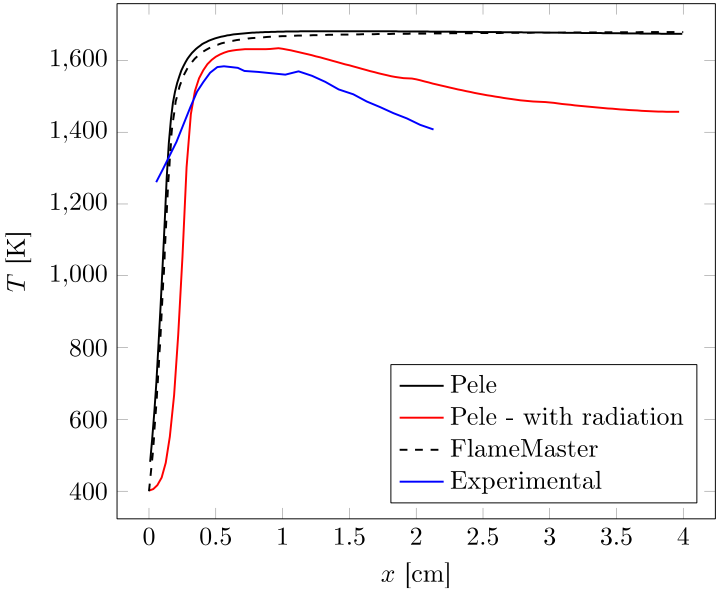


16 m/s jet in 72 m/s air crossflow using KHRT breakup model

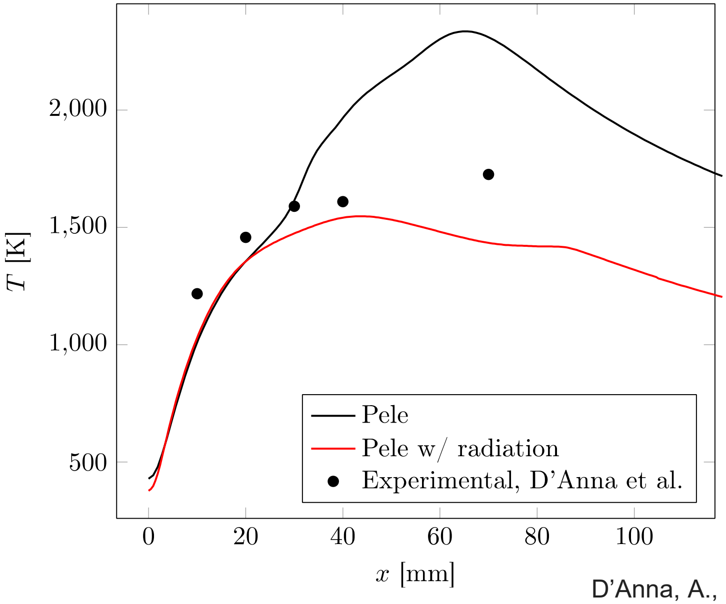
Lui, A., et al. *SAE Technical Paper* 930072 (1993)

- KHRT breakup model
  - Patterson, M. A. and Reitz, R. D. (1998)
  - Verification using jet in crossflow configuration
- ETAB breakup model
  - O'Rourke, P. J. and Amsden, A. A. (1987)
  - Tanner, F. (1997)
- Splash model
  - Ahamed, S. et al. (2022)
- Wall film evaporation model
  - O'Rourke, P. and Amsden, A. A. (1996)

Soot and Radiation Modeling

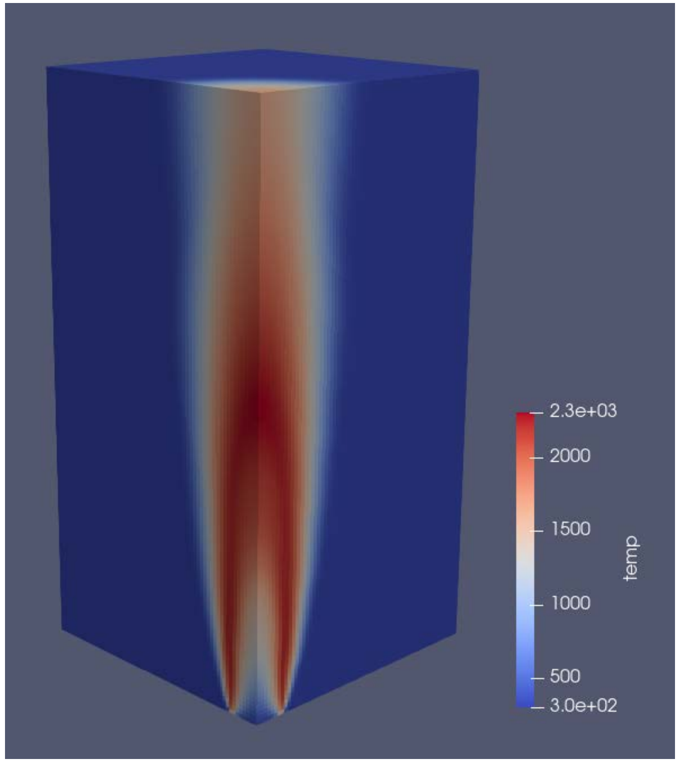


Ethylene 1D burner simulation



D'Anna, A., et al. (2004)

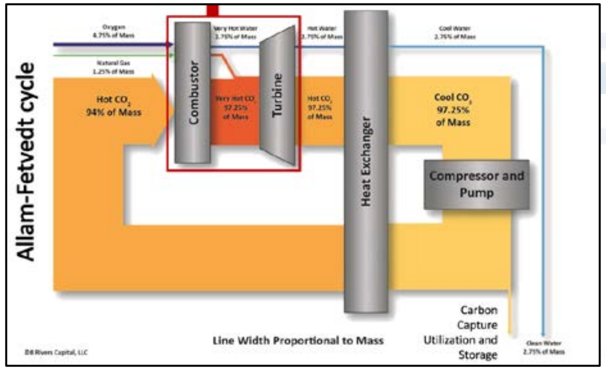
Ethylene co-flow centerline temperature



Ethylene 3D co-flow temperature

- Eulerian hybrid method of moments (HMOM)
    - Mueller et al. Combust. Flame (2009)
- Requires precursor chemical species in chemical mechanism – pyrene, napthalene
- Radiation: P1 gray gas model and the Planck-mean spectral model for the gas products and soot

Beyond PELE’s Stretch Goals



Reacting flows are an integral part of key technologies for the energy transition and circular economy for materials

- Sustainable aviation
- Oxy-combustion w/ Carbon sequestration
- Biomass processing
- Pyrolytic recycling of polymers
- Green steel, cement and chemical production

Simulations are necessary to advance and deploy these technologies

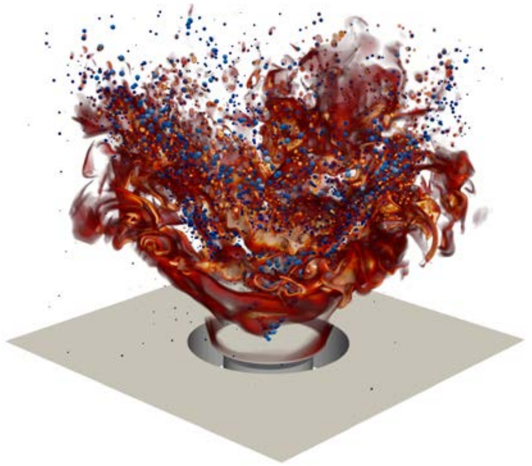
- Exascale computing: unprecedented ability for high-fidelity simulation, generating immense volumes of data
- Evaluation of chemical kinetics can be >90% of computational intensity

Objective: use data generated from exascale scientific simulations to generate low-cost models that can be used to accelerate engineering calculations

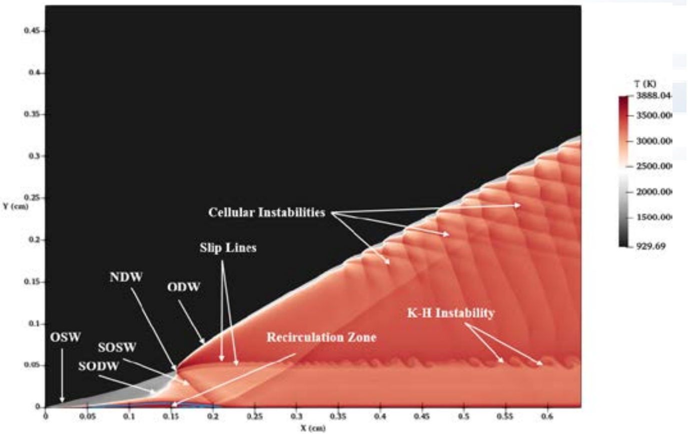
PeleC and PeleLMeX community code for turbulent reacting flows with multi-physics addressing climate mitigation and national security challenges

- Certifying sustainable aviation fuels for propulsion
- Enabling clean efficient dispatchable power generation with hydrogen and hydrogen blends in existing infrastructure
- Enabling chemical manufacturing with low energy heat sources from plasma catalysis (DOE Industrial Heat Shot Earthshot)
- Creating digital twins of hypersonic nonequilibrium reacting flows
- Reliably powering unmanned aerial systems with fuel diversity

Complex multi-physics insights in reactive flows and high-fidelity data for reduced-order models



Aero-engine spray flame stabilization with SAF fuel (C1-ATJ)



Mach 10 oblique detonation with nonequilibrium H_2/O_2 chemistry

Scramjet cavity stabilized flame

EXASCALE COMPUTING PROJECT

LES Models in PeleLMeX

- Subfilter momentum and scalar transport terms closed with gradient-transport models:

Scalars

$$\bar\rho\widetilde{u_j\phi} - \bar\rho\tilde{u}_j\tilde{\phi} = -\frac{\mu_t}{\mathrm{Sc}_t}\frac{\partial\tilde{\phi}}{\partial x_j}$$

Momentum

$$\tau_{ij} = (\bar\rho\widetilde{u_i u_j} - \bar\rho\tilde{u}_i\tilde{u}_j)\,, \qquad \tilde{S}_{ij} = 1/2\left(\frac{\partial\tilde{u}_i}{\partial x_i} + \frac{\partial\tilde{u}}{\partial x_j}\right)$$

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_i j \approx -2\mu_t\left(\tilde{S}_{ij} - \frac{1}{3}\delta_{ij}\tilde{S}_{kk}\right)$$

- Smagorinsky and Wall-Adapting Local Eddy Viscosity (WALE)[1] models implemented in PeleLMeX

Smagorinsky

$$\mu_t = (C_s\bar{\Delta})^2|\tilde{S}|$$

Nominal Value:
$C_s = 0.18$ (Cs1x)
Also evaluate:
$C_s = 0.09$ (Cs0.5x)
$C_s = 0.36$ (Cs2x)

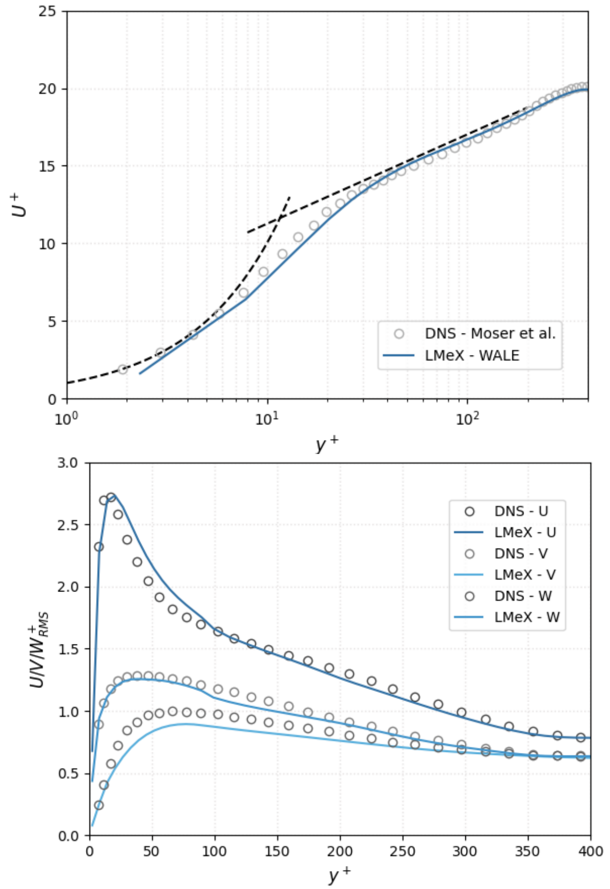
WALE

$$\tilde{S}^d_{ij} = \frac{1}{2}\left(\left(\frac{\partial\tilde{u}_i}{\partial x_j}\right)^2 + \left(\frac{\partial\tilde{u}_j}{\partial x_i}\right)^2\right) - \frac{\delta_{ij}}{3}\left(\frac{\partial\tilde{u}_k}{\partial x_k}\right)^2$$

$$\mu_t = (C_m\bar{\Delta})^2\frac{\left(\tilde{S}^d_{ij}\tilde{S}^d_{ij}\right)^{3/2}}{\left(\tilde{S}_{ij}\tilde{S}_{ij}\right)^{5/4} + \left(\tilde{S}^d_{ij}\tilde{S}^d_{ij}\right)^{5/2}}$$

$C_m = 0.60$

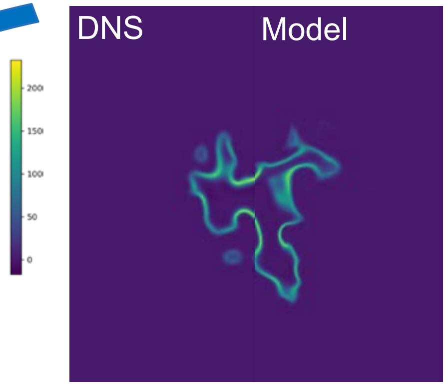
Basic validation: 1D Channel Flow



[1] F. Ducros, F. Nicoud, and T. Poinsot. *Numerical Methods for Fluid Dynamics VI* (1998) 293-299.

Manifold Models & ML in Pele

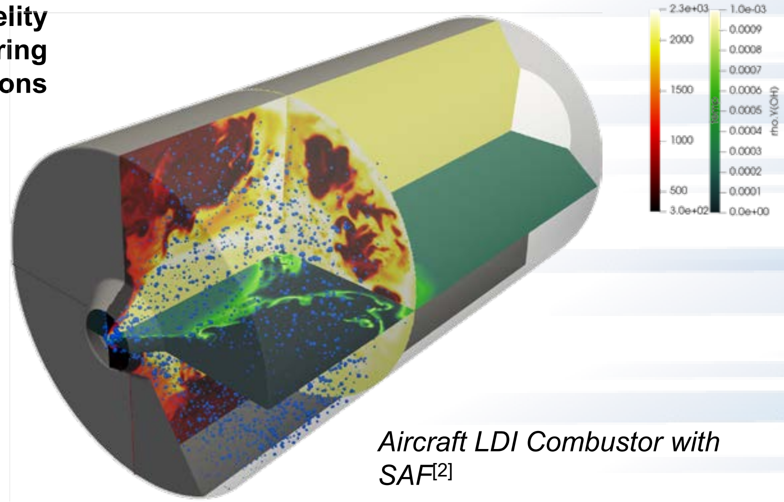
Direct Numerical Simulations (DNS) using PeleC & PeleLMeX ->TB of data



Ex. Turbulent ignition of Jet-A
(A. Krisman, J. Chen, SNL w/S3D)

Closing the loop:
A Posteriori
validation

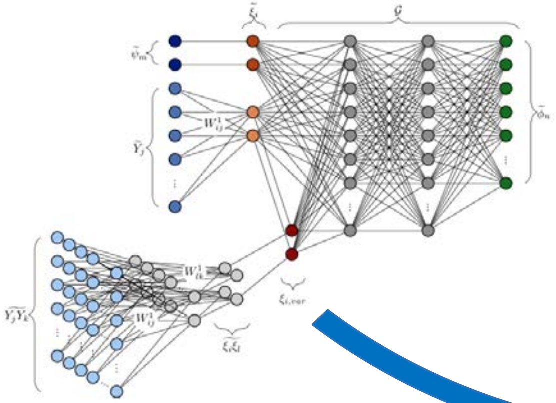
High-Fidelity Engineering Calculations

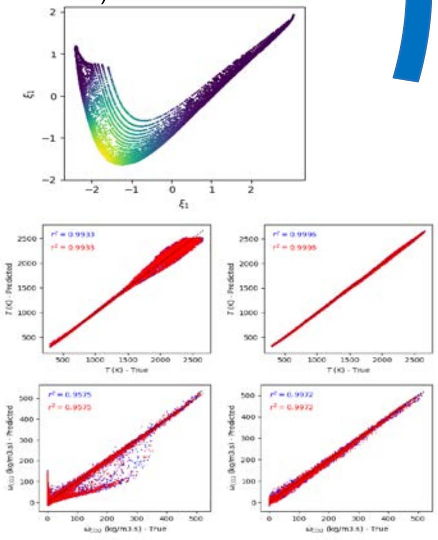


Aircraft LDI Combustor with SAF[2]

ML Model Training

Ex.: Co-optimized Machine-Learned Manifolds[1]





A Priori **Model Validation**

Leverage data from high-fidelity simulations to improve reduced-order manifold chemistry models

Implement reduced-order manifold capability in Pele codes to enable a posteriori validation and engineering simulations, e.g. for SAF combustion

General Implementation: Allow for both physics- and data-based manifolds

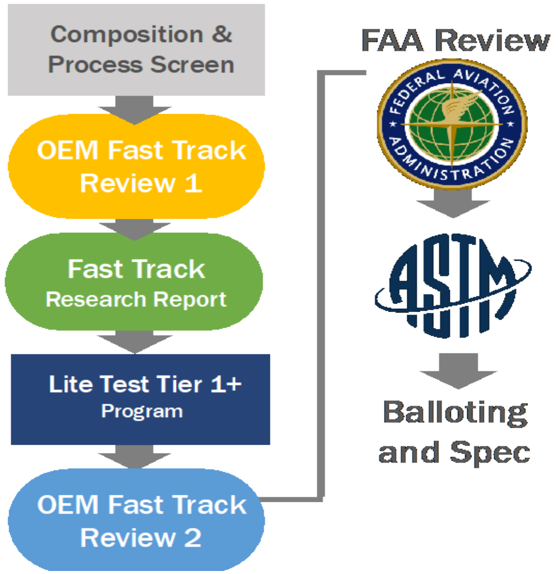
[1] B.A. Perry, M.T. Henry de Frahan, S. Yellapantula. Combustion and Flame 244C (2022) 112286

[2] Sreejith N.A., et al. 13th U.S. National Combustion Meeting (2023) Paper #2C07

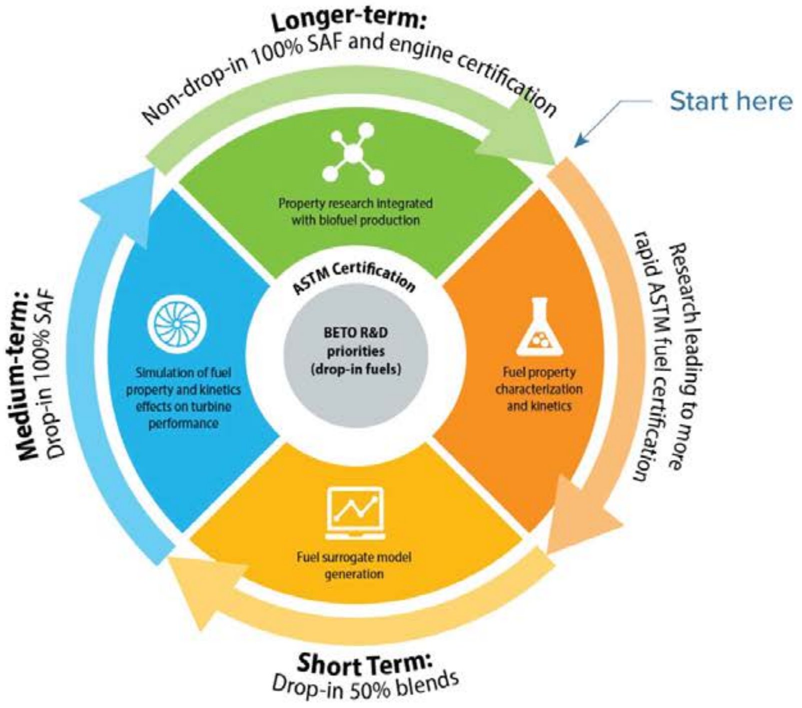
Supporting Decarbonization of Aviation

New ASTM “Fast Track” Approval Process in 2020

<1k gal, <$1M, <2 years



The SAF technology landscape

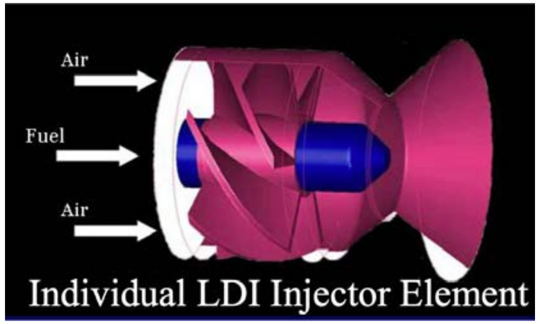


BETO VTO

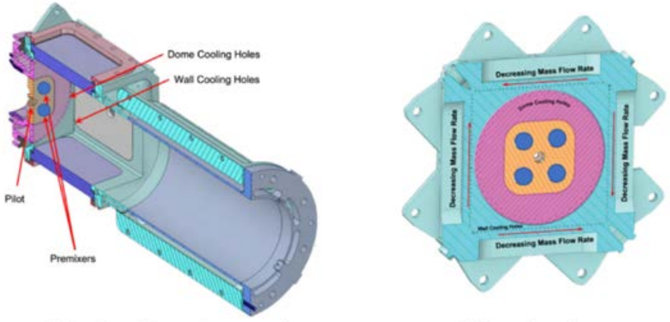
- Fuel production: BETO
- Fuel property characterization: BETO and VTO
- Fuel property mapping to turbine performance: VTO
- Expanding boundaries of ASTM certification: VTO
- De-risking qualification of new fuels (drop-in and marginally drop in): VTO and BETO

SAF Fuel Effects in Aero Combustors

NASA – Lean Direct Injection (LDI)
7 element configuration



Lean premixed pre-vaporized (LPP) design for commercial supersonic transport (CST)

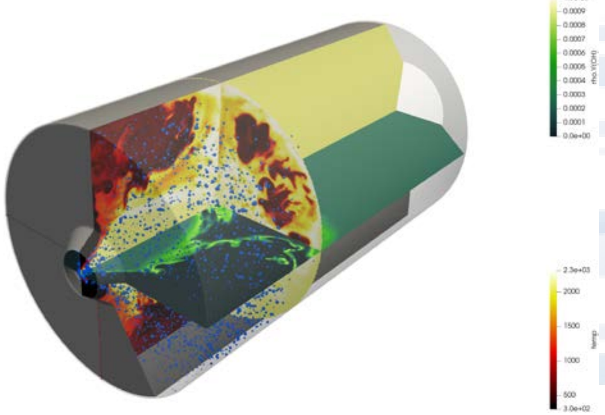


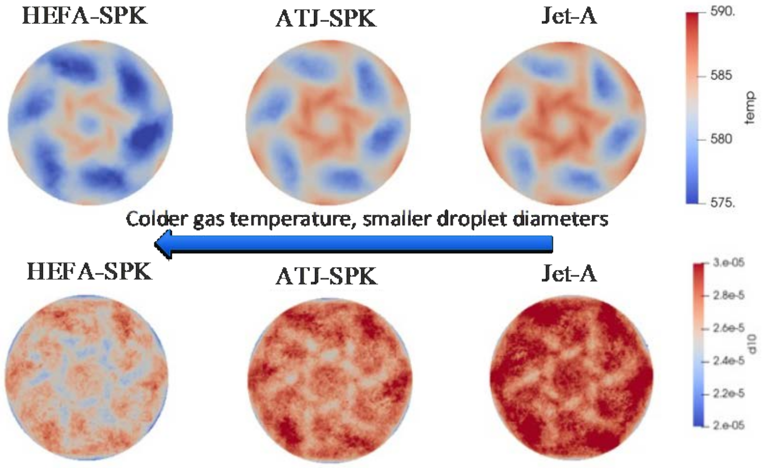
(a) Cut-view of the combustor test rig

(b) Front dome plate

Combustor concept under development at GE Aviation and Georgia Tech – Funded by FAA

T3 = 600 K (~620°F)
P3 = 20 bar (~300 psia)

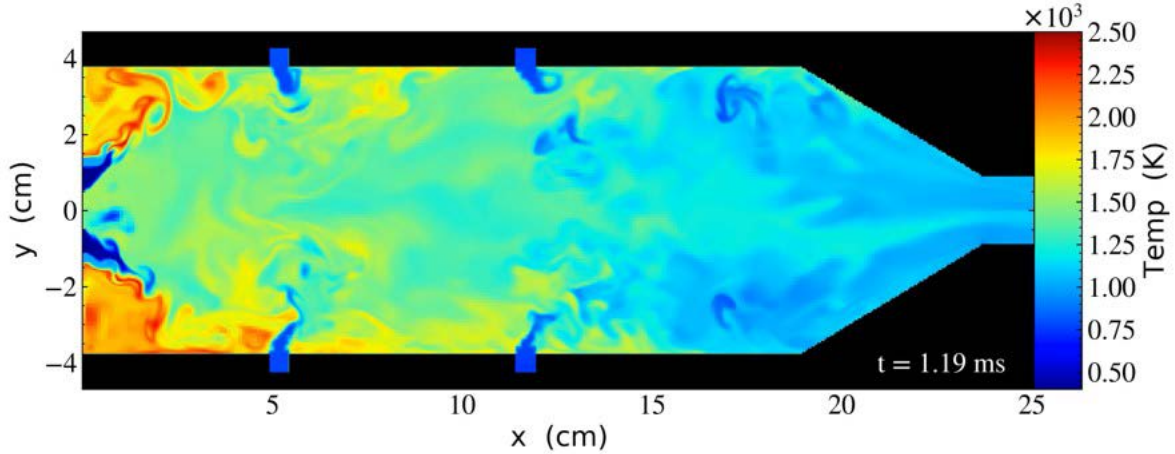




Differences in viscosity and surface tension of HEFA-SPK lead to significant difference vaporization characteristics when compared against Jet-A

Decarbonization of Power Generation

PeleC simulation-based study of 50 MW oxy-combustor developed by NET Power (8 Rivers, LLC)

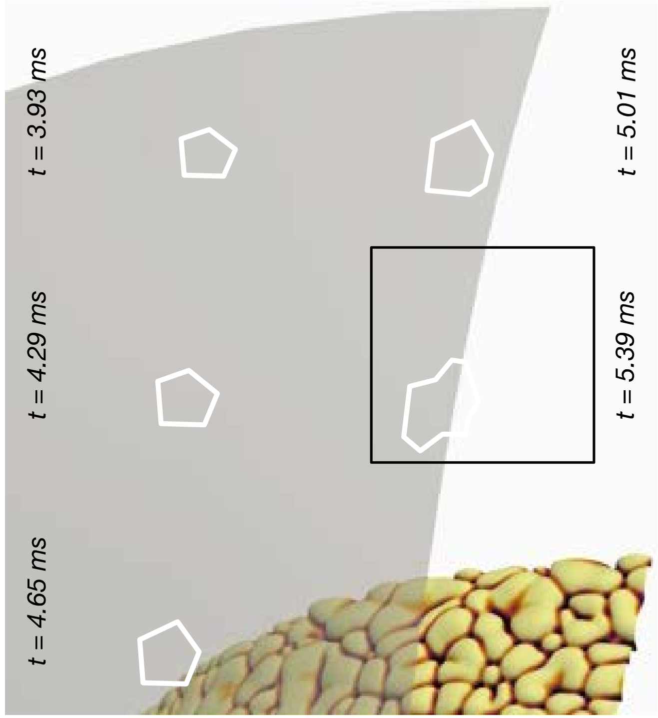


Oxycombustion concept from NET Power (8 Rivers LLC)

- Allam-Fetvedt Cycle for supercritical CO2
- Almost complete carbon capture
- NG (fuel) + O2 (oxidizer) + CO2 from dilution holes
- CO2 concentration > 0.8 (vs. 0.1 traditional)
- Operating pressure: 300 bar!
- Supercritical conditions require Soave-Redlich-Kwong EOS model (vs. ideal gas)
  - Strong impacts on density models, transport and chemistry

Geometry based on the 50MW demo being run by NET Power since 2019 in Texas. Simulations were performed at part load to help NET Power with combustor design.

Fundamental and applied research on hydrogen combustion for power generation



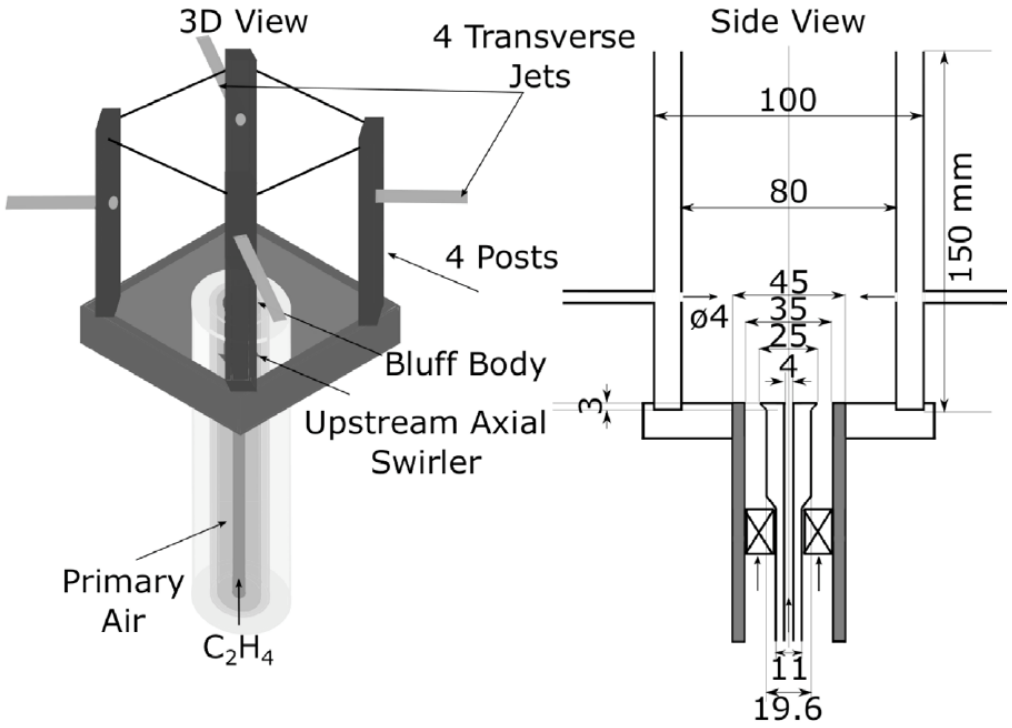
PeleLM study of Darrieus-Landau (hydrodynamic) and thermo-diffusive instabilities in hydrogen flames

Advanced fuel nozzle simulations using PeleC for high H2-CH4 fuel blends to avoid flashback in stationary gas turbines

High-fidelity Pele simulation of a lab-scale combustor with sustainable aviation fuels (C1 comparison with Jet-A)

Cambridge swirl-stabilized spray flame

- El Helou et al (2023) *Fuel* https://doi.org/10.1016/j.fuel.2022.125608
- Study soot formation: Jet-A and C5



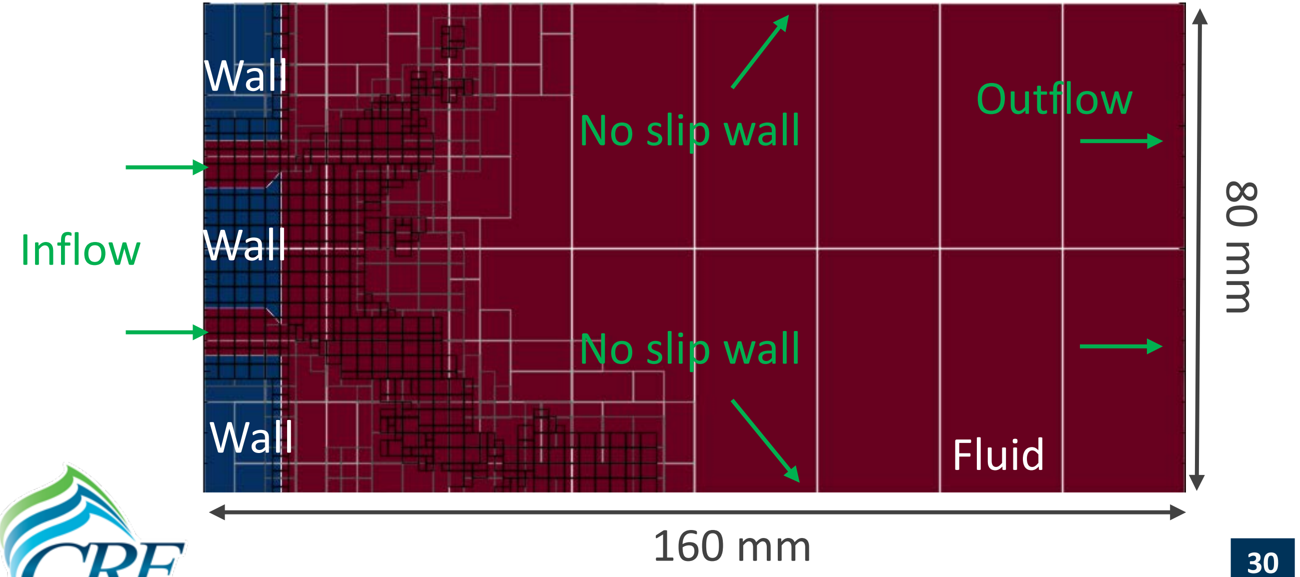
PeleLMeX physical and numerical parameters

- Lagrangian multi-phase spray model
- Embedded boundary treatment
- 4 AMR levels (base + 3 levels): dx = 78 μm. Number of cells: approx. 350M

Targeted fuels

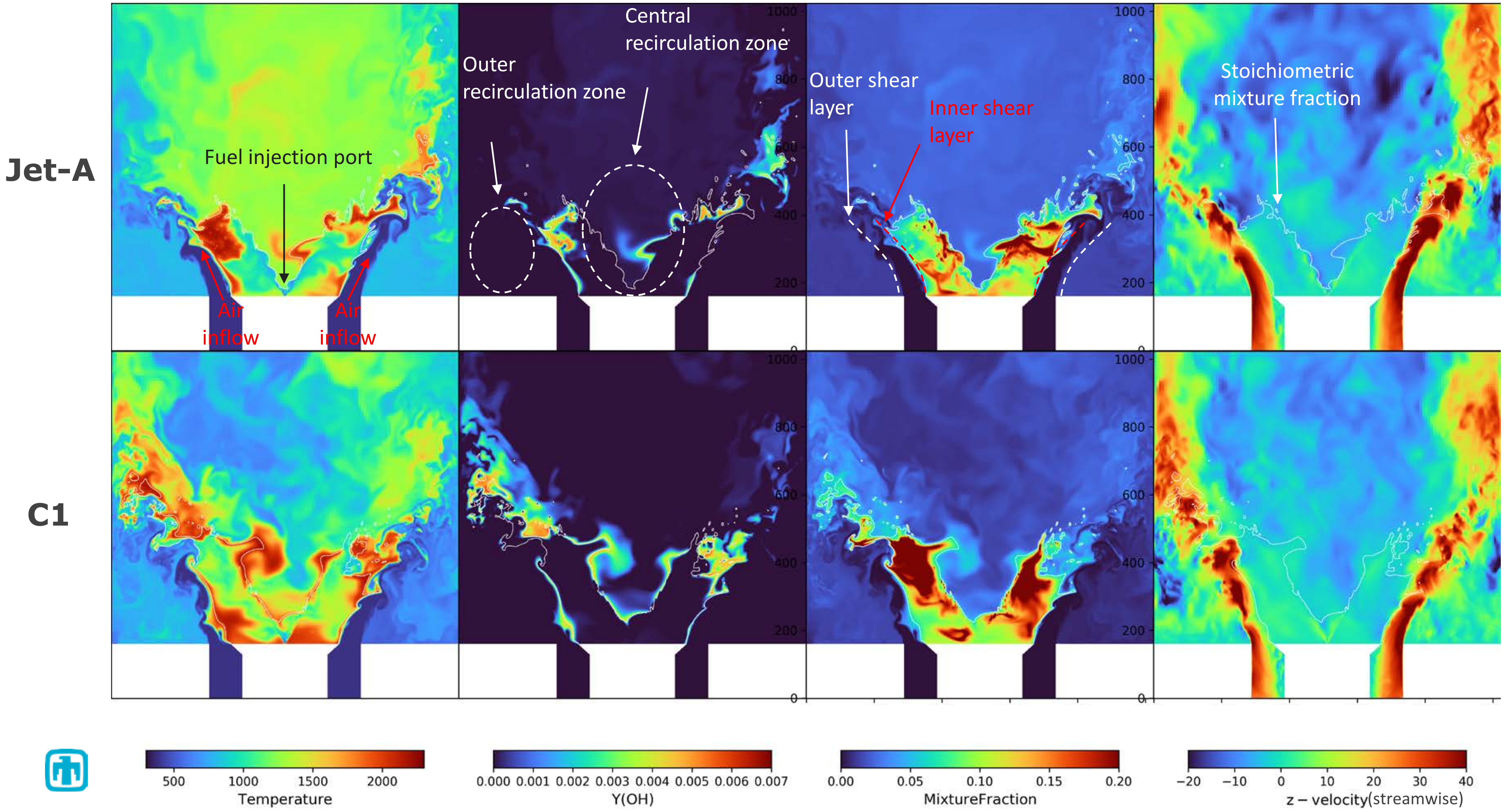
  - Jet-A: 48-species UIUC mech (Ryu et al. 2021)
  - C1: 57-species UIUC mech (Kim et al. 2021)

PeleLMeX set up with AMR grid



B. Soriano, et al. 2023 (in prep)

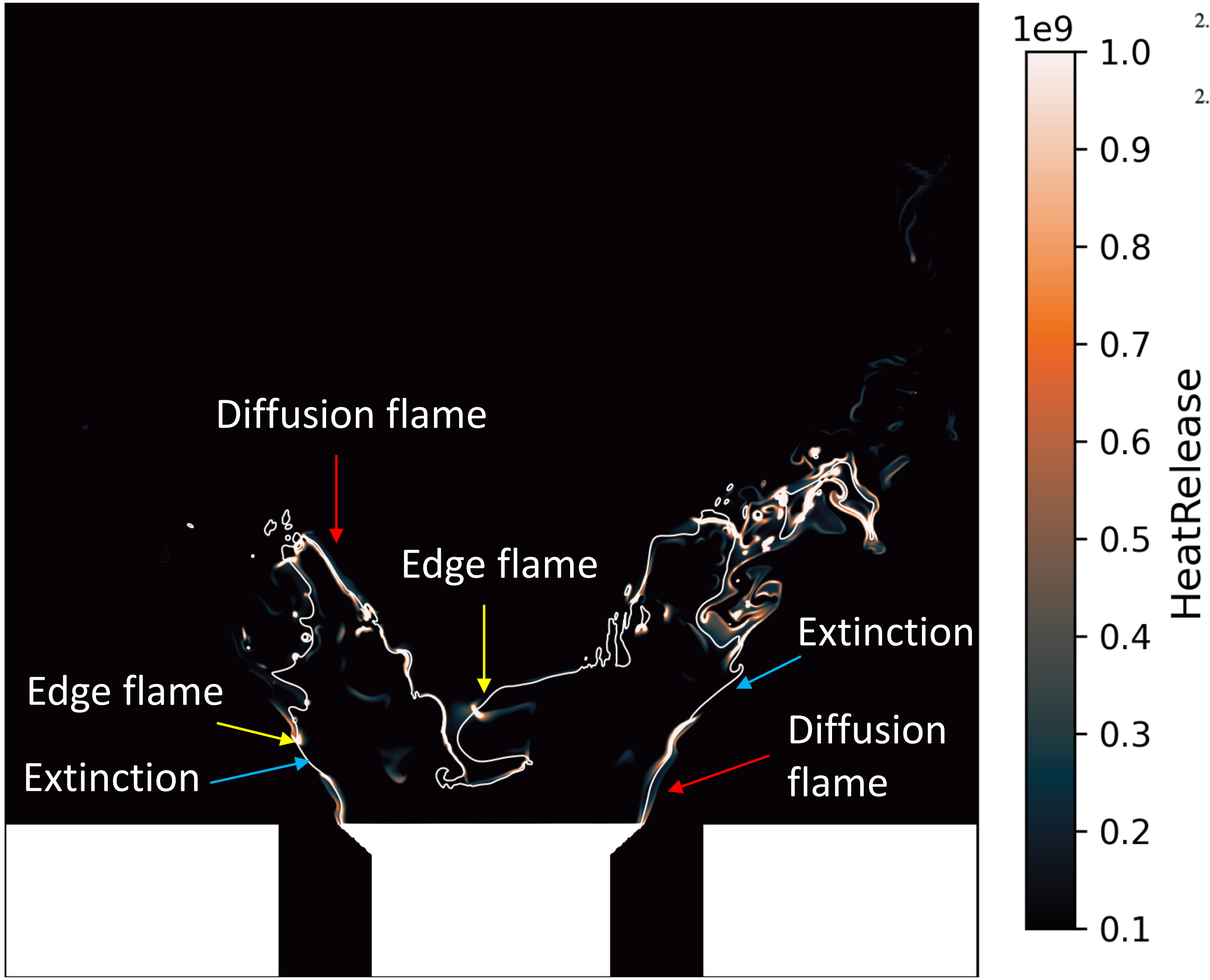
Instantaneous flame behavior for Jet-A and C1



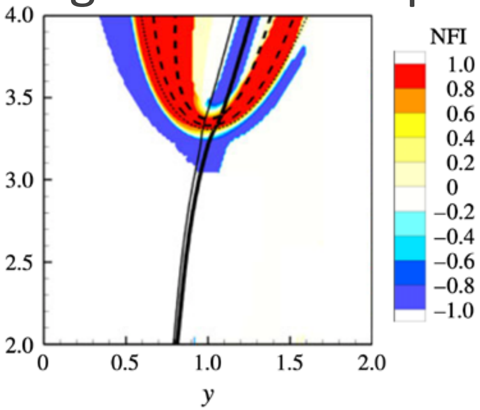
Instantaneous Heat Release Rate for Jet-A

Complex flame behavior
- Diffusion flame
- Local extinction
- Edge flame propagation

Is the edge flame a deflagration front or an ignition front?



Edge flame example



Karami et al. J. Fluid Mech. (2015), vol. 777, pp. 633–689.

Quantification of ignition/deflagration for Jet-A and C1

Damköhler number can be used to quantify deflagration fronts

$$Da = \frac{\dot{\omega}_k}{|-\nabla(\rho Y_k V_k)|}$$

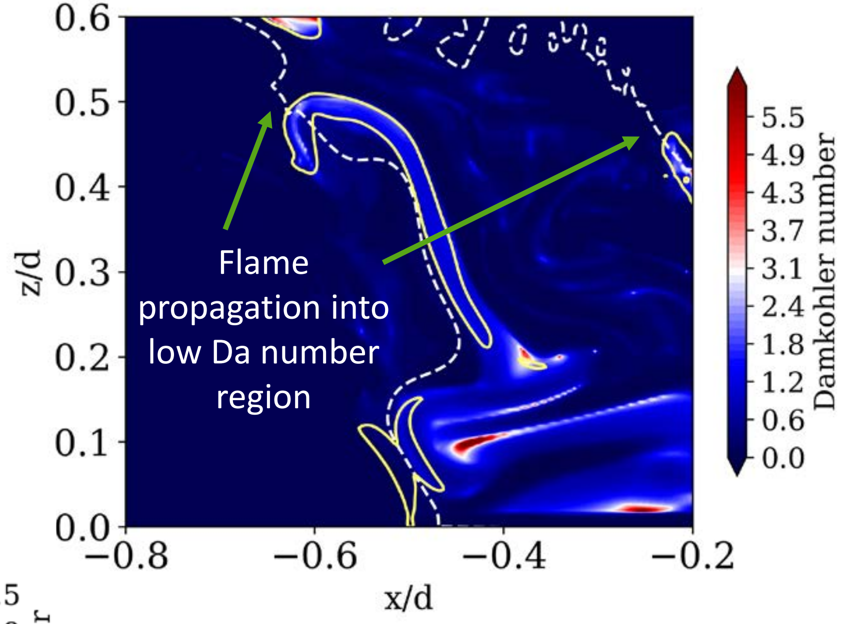
$$Y_c \equiv Y_{CO_2} + Y_{CO}$$

Damköhler number is typically around 3[1]

Da > 3 => ignition

Da < 3 => diffusion limit

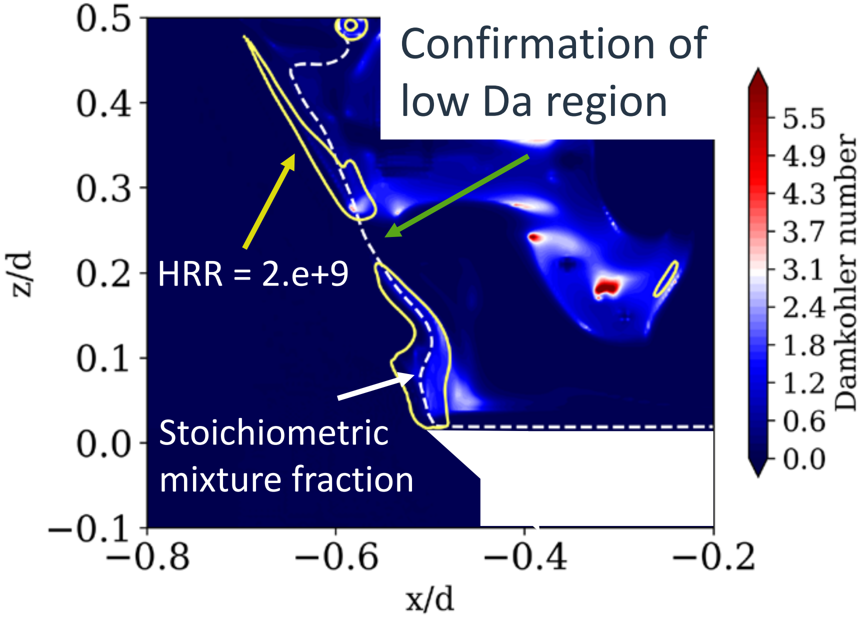
C1



Flame propagation into low Da number region

Jet-A

Inner shear layer

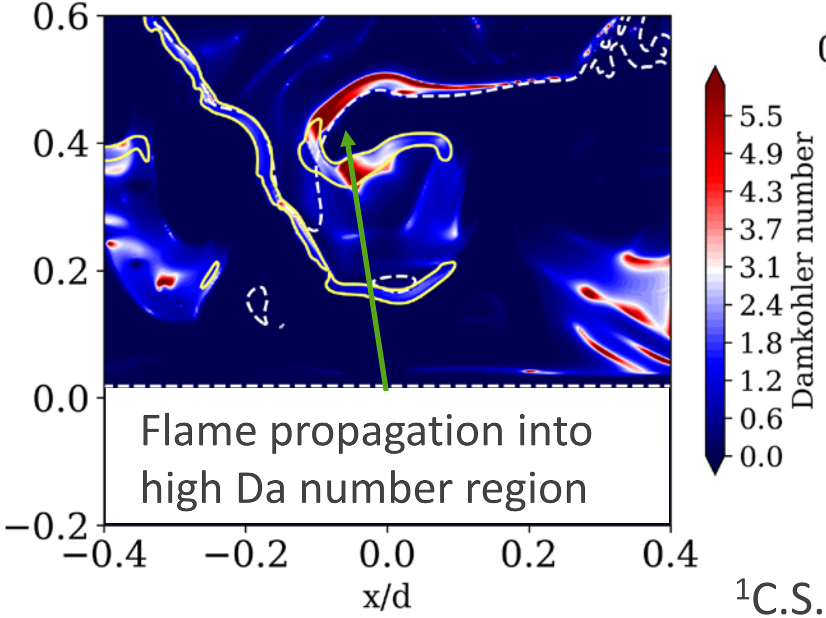


Confirmation of low Da region

HRR = 2.e+9

Stoichiometric mixture fraction

Central recirculation near fuel injection



Flame propagation into high Da number region

- Deflagration and ignition fronts coexist!
- Ignition effects more pronounced for Jet-A

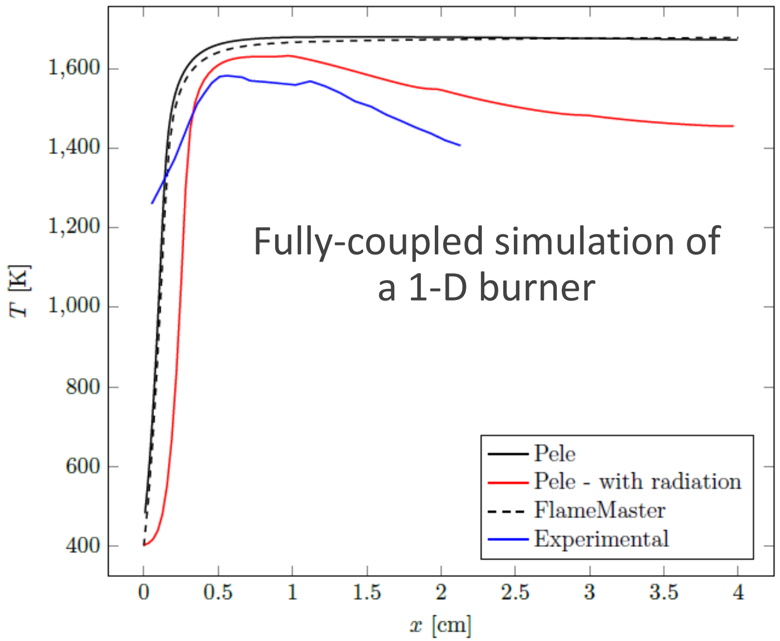
---

[1] C.S. Yoo et al. PROCI 34 (2013) 2985–2993

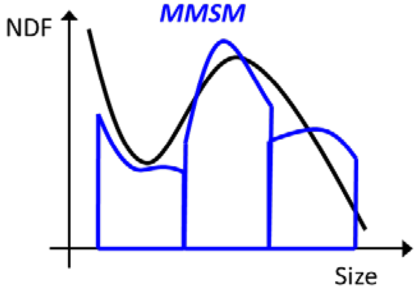
Future work

- **Short-term:**
  - ❑ Cambridge burner with soot predictions and radiation
    - ▪ Soot: Hybrid method of moments (HMOM) soot model
      - Focus on soot oxidation
    - ▪ Radiation: P1 gray gas model and the Planck-mean spectral model for the gas products and soot
- **Mid-term:**
  - ❑ Simulations at high pressure
- **Long-term:**
  - ❑ New Approach for soot modeling: Multi-Moment Sectional Method (collaboration with M. Mueller)

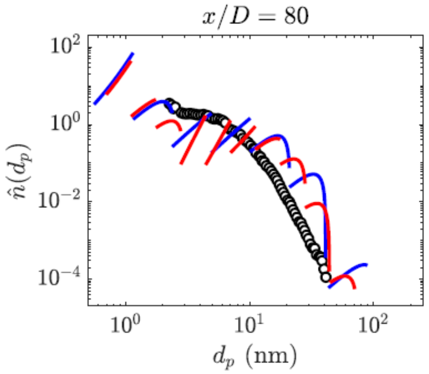
Validation of Pele implementation of soot model and radiation



Fully-coupled simulation of a 1-D burner



Bivariate MMSM[2] + Large Eddy Simulation[3]



Basic Idea[1]: Fewer sections with local polynomial approximation of size distribution within each section

- Converges faster than sectional method
- Many fewer degrees-of-freedom required compared to sectional method

---

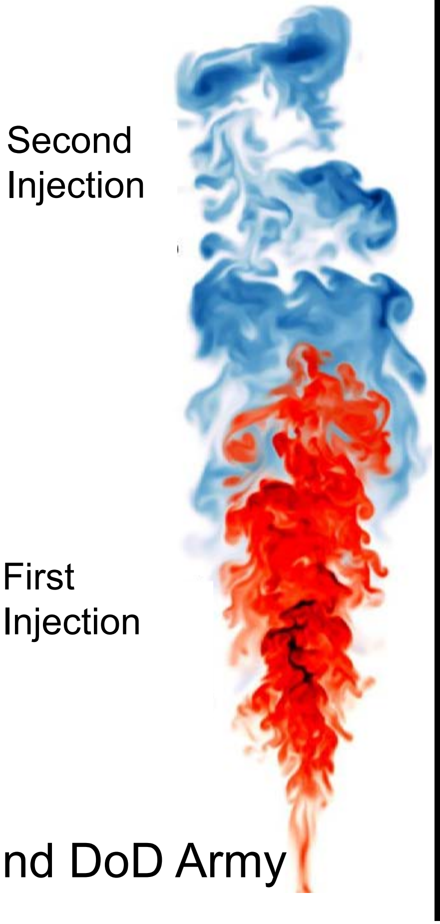
[1] S. Yang, M.E. Mueller, Proc. Combust. Inst. 37 (2019) 1041-1048

[2] H. Maldonado Colmán, M.E. Mueller, 18th International Conference on Numerical Combustion , 2022

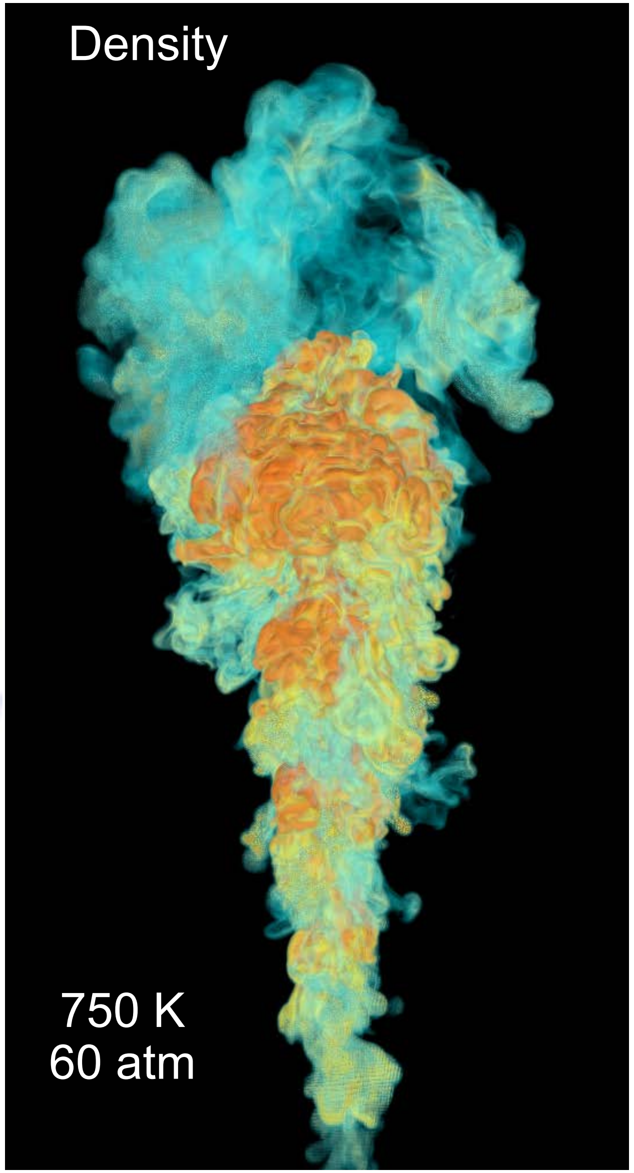
[3] H. Maldonado Colmán, M.E. Mueller, 13th U.S. National Combustion Meeting, 2023

DNS of multi-injection diesel jet flames (PeleLMeX) ndodecane and SAFS

- Simplified gaseous pre-vaporized jets, down-scaled compared to experiment (reduced Re, same Damkohler number)
- Low-Mach jets simulated with PeleLM
- 35 species n-dodecane mechanism with both 1st and 2nd stage ignition chemistry (Borghesi et al., 2018, based on Yao et al., 2017)
- Up to ~3B grid cells, run on Cori
- Simulated two cases at 750 and 900 K oxidizer temperature at 60 atm, 15% O_2 in oxidizer
- Data is used for understanding of physics, and for evaluation and improvement/development of engineering-type models
  - insight into mechanism behind experimental observations of 1st-stage combustion products of first injection affecting ignition of second injection (mixing with high temperature products of first-injection combustion, or mixing with radical species, or flame propagation into penetrating second injection?)



N-dodecane multi-injection



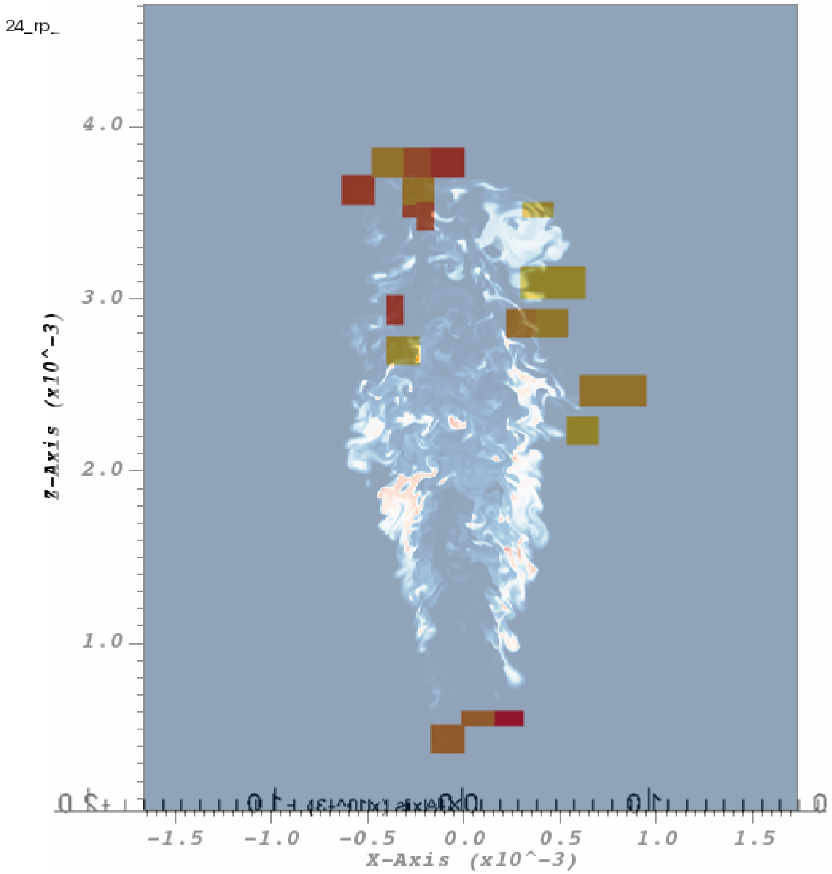
Sponsors: DOE Vehicle Technologies Office and DoD Army

Detection of anomalies using AI/ML (Pele – ALPINE – ExaLearn Integration KPP3) for Physics Discovery and steering

- Summary: AI/ML techniques independently developed in ExaLearn are being deployed in-situ with Ascent technology from ALPINE to detect auto-ignition regions in a PeleLM simulation.
- Part of a sustained integration effort through 2023 to explore engine knock
  - KPP-3 goals for ALPINE/ExaLearn, in support of Pele goals:
    - Functionality: in situ anomaly detection as a trigger for further analysis
    - Applications: Turbulent combustion + Higher-order moment tensor analyses
    - Technologies: PeleLM, Ascent, Genten
    - Platform: Summit
- Current Status:
  - PeleLM KPP-2 simulation on Frontier (reactivity controlled pulsed ignition of diesel fuel) coupled with Ascent/Genten libraries for in-situ ignition detection.
  - Necessary components of PeleLM (boundary conditions, chemistry modules) are GPU-ready.

- Long-term Pele goals served by this integration:
  - In-situ reduced order modelling for chemistry dimension reduction.
  - Targeted DNS training data for constructing PINNs, hybrid ROMs.

Simulation snapshot of an intermediate species overlaid with AMR boxes flagged by the anomaly detection algorithm



C12H24 (density)

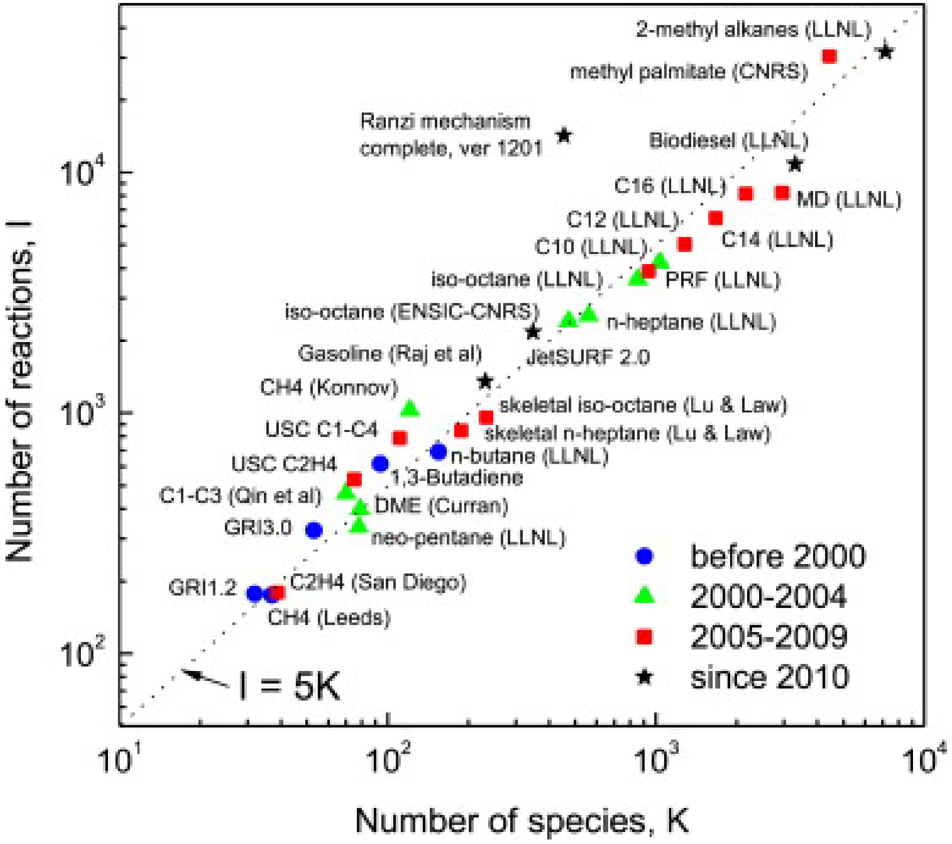
Contributors: Martin Rieth, Jackie Chen (Pele), Marco Arienti, Matt Larsen, Janine Bennett (ALPINE), Hemanth Kolla (ExaLearn)

Motivation

Direct Numerical Simulation (DNS)

Advantages:
- **Full access to time/space resolved 3D fields**

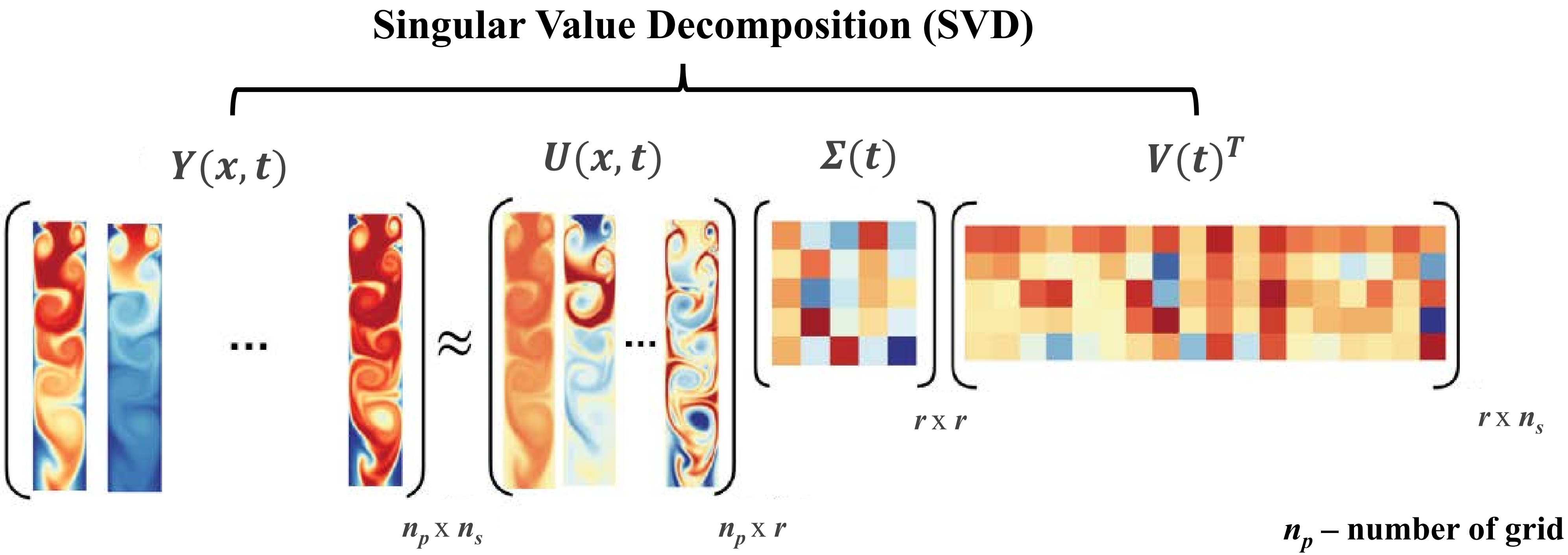
Disadvantages:
- **Huge computing and memory requirements**



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
  - Domain expertise (Offline cost)

1: Egolfopoulos et al., Prog. Energ. Combust., 2014

Dynamical bi-orthonormal (DBO) decomposition-based ROM



n_p – number of grid points
r – reduction size
n_s - number of species ($r \ll n_s$), doesn't include the bath gas

Idea: Obtain on-the-fly low-rank decomposition of species transport equation[1,2]

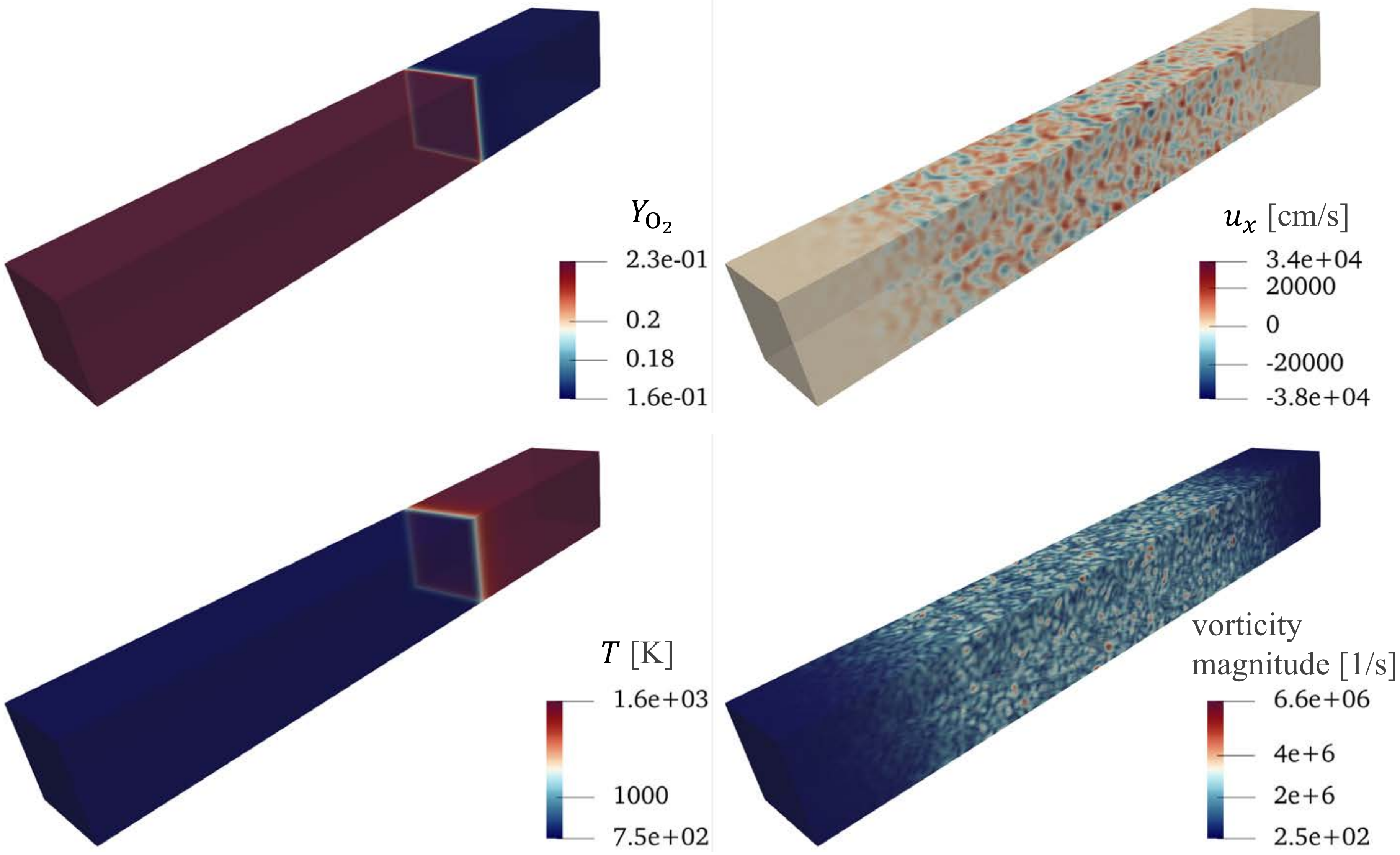
Advantages:

- No need to generate training data
- 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

1: Patil et al., JCP 2020
2: D. Ramezanian et al., Comp. Met. Appl. Mech. & Eng., 2021

Test Case: 3D turbulent flame propagation of a lean premixed hydrogen/air mixture

Initial fields:



Initial Condition:

$\phi = 0.3$
$T_u = 750$ K
$p = 1$ bar
$u'/s_l = 21.3$
$l_t/\delta_l = 2.25$
$Re_t = 1{,}000$
$Ka = 300$
$L_x \times L_y \times L_z =$
$1.69 \times 0.226 \times 0.226$ cm^3

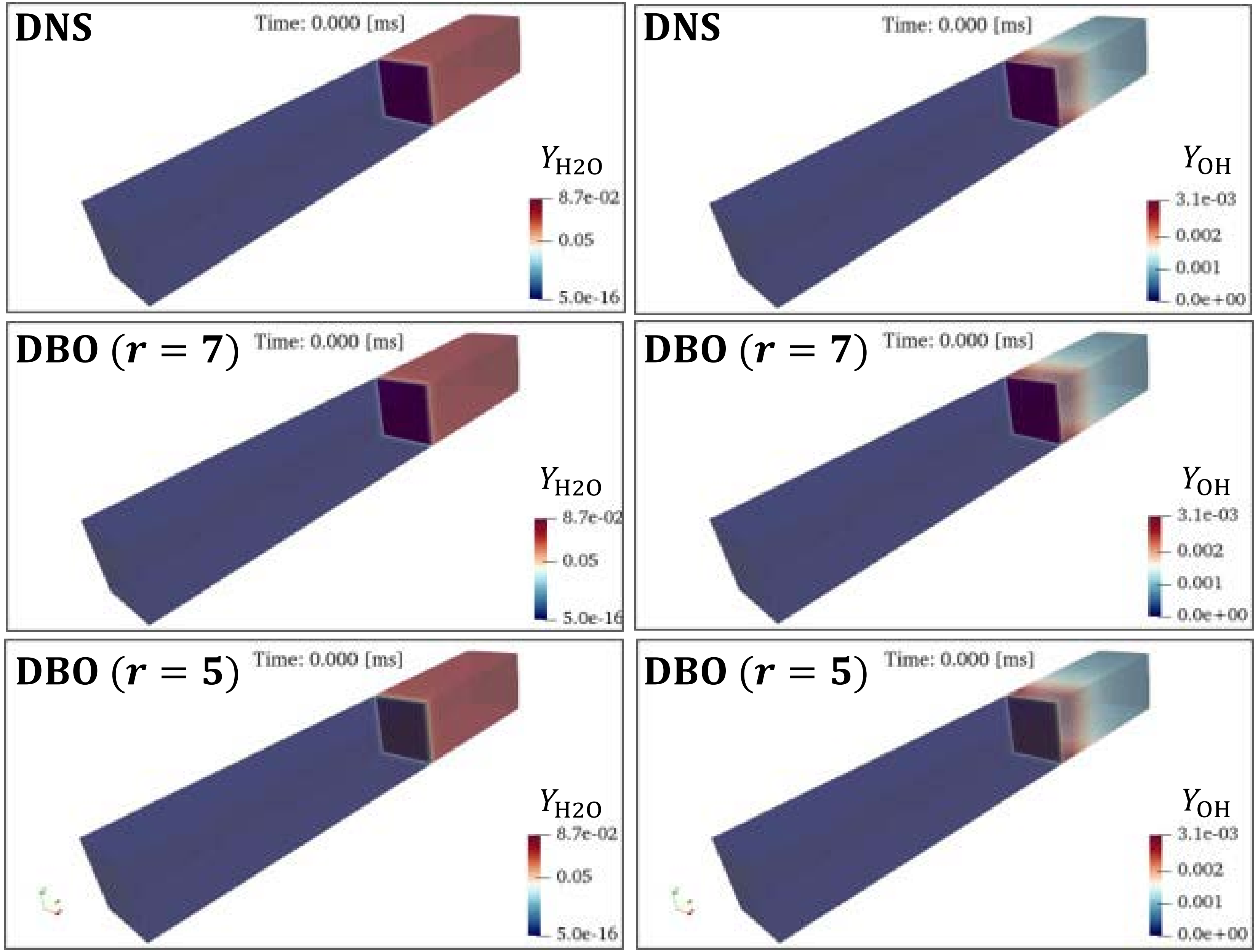
30-micron grid resolution (coarser grid)

9-species detailed H_2/air mechanism

Initialized by 1-D freely-propagating laminar flame

DBO-ROM with $r = 5$ or 7 started at $t = 0$

Test Case: 3D turbulent flame propagation of a lean premixed hydrogen/air mixture



The initial laminar flame structure is transitions to a turbulent flame due to the superimposed isotropic turbulence field

The isotropic turbulence dissipates with time → flame wrinkling ↓ with time

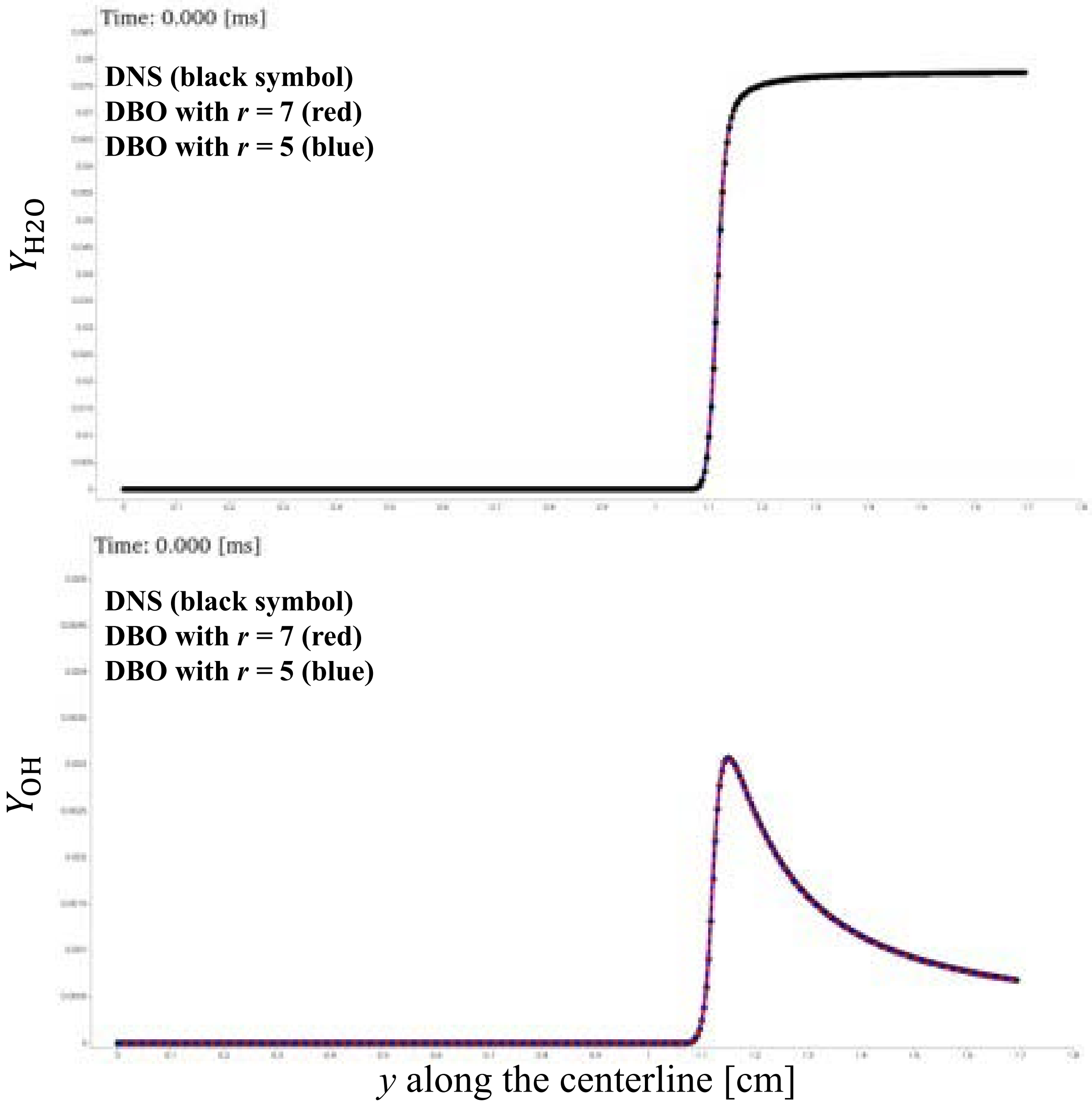
DBO with rank = 7 accurately captures the temporal evolution of major and minor species

DBO with rank = 5 fails to capture the flame propagation characteristics of the hydrogen/air mixture (fuel consumption speed is underestimated)

9-species detailed H_2/air mechanism is an inherently a high-dimensional system → difficult to apply reduced-order modelling

Test Case: 3D turbulent flame propagation of a lean premixed hydrogen/air mixture

Temporal evolution of mass fraction of H_2O and OH along the centerline ($x = L_x/2$, $z = L_z/2$)



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9-species detailed H_2/air mechanism is inherently high-dimensional system → difficult to apply reduced-order modelling

Thank you!

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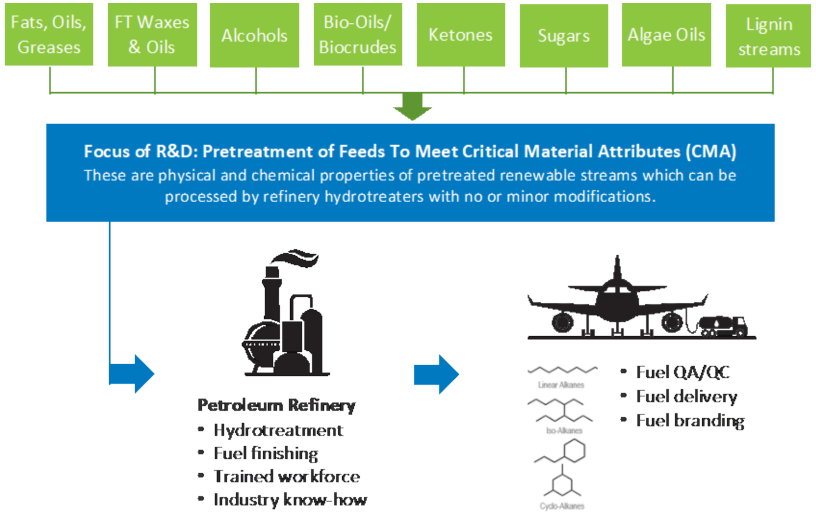
NREL/PR-2C00-85968

This work was authored in part by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by U.S. Department of Energy Office of Science and National Nuclear Security Administration. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes. This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration. A portion of the research was performed using computational resources sponsored by the Department of Energy's Office of Energy Efficiency and Renewable Energy and located at the National Renewable Energy Laboratory. This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725.

NREL

Transforming ENERGY

NREL Bio-Fuel Property Measurement



Fats, Oils, Greases | FT Waxes & Oils | Alcohols | Bio-Oils/ Biocrudes | Ketones | Sugars | Algae Oils | Lignin streams

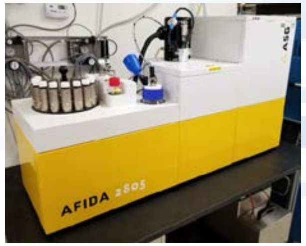
Focus of R&D: Pretreatment of Feeds To Meet Critical Material Attributes (CMA)
These are physical and chemical properties of pretreated renewable streams which can be processed by refinery hydrotreaters with no or minor modifications.

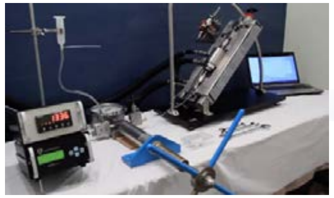
Petroleum Refinery
- Hydrotreatment
- Fuel finishing
- Trained workforce
- Industry know-how

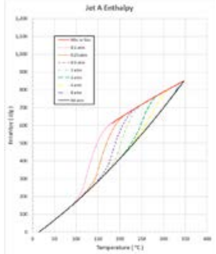
- Fuel QA/QC
- Fuel delivery
- Fuel branding

Anton Paar Viscometer

NanoScience Surface Tension







Soon to be commissioned:

Viscosity at 68 bar and -40°C to 315°C
Density at 500 bar and -10°C to 110°C
Surface Tension at 68 atm and -35°C to 450°C
Ignition delay with AFIDA
Pressure-enthalpy diagram by DSC