MARCH 16TH, 2025

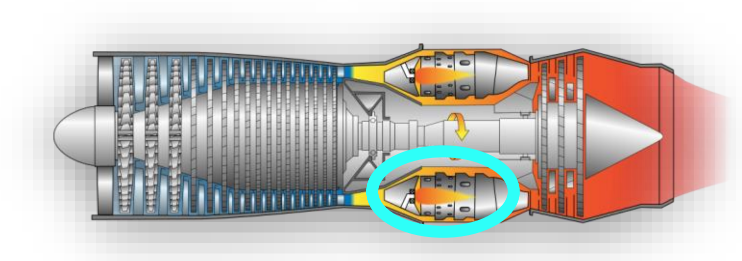
ENABLING FUEL-FLEXIBLE PROPULSION AND POWER GENERATION DEVICES BY LEVERAGING LEADERSHIP COMPUTING AND HIGH-FIDELITY EXPERIMENTS

SIBENDU SOM
Director – Advanced Propulsion and Power Department

Carbon-Free Fuel Workshop @ NCM 2025

OVERVIEW

- ❑ Big Science Tools/Core Capabilities
  - Leadership computing (Exascale)
  - Advanced Photon Source – x-ray diagnostic
  - Technology transfer to industry
- ❑ Recip. Engines
  - DNS, LES, RANS, & ROMs for optimization
  - Challenges and opportunities with H2-ICE
- ❑ Gas turbines
  - SAF end-use research
  - Film cooling
- ❑ Other applications: RDE, Stationary Power generation, High-speed flows, Burners, …
- ❑ Concluding remarks



*Conceptual Rendering

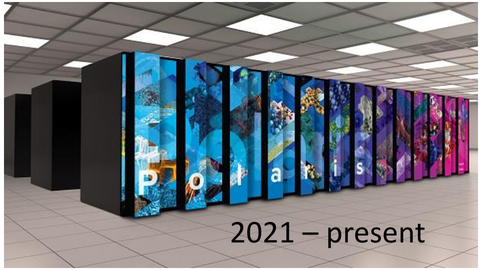
BIG SCIENCE TOOLS/CORE CAPABILITIES

- LEADERSHIP (EXASCALE) COMPUTING
  - Nek5000 CODE FOR DNS/LES
- ADVANCED PHOTON SOURCE

LEADERSHIP (EXASCALE) COMPUTING

Nek5000/nekRS: Exascale ready code

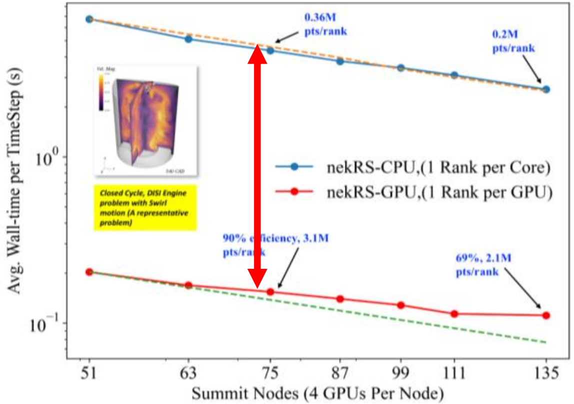
Theta/Theta-GPU



Polaris (GPU only)

Aurora: Exascale Machine

- **High-order in space (spectral element method, 5th - 15th order) and in time (up to 3rd order)**
- nekRS - the GPU variant of Nek5000
  - **GPU-ready exascale** codes under active development leveraging ~$15M ASCR investment
  - **Scales on ~30,000 GPUs**
- Nek5000/NekRS codes used to perform high-fidelity device-level simulations to benchmark/train models

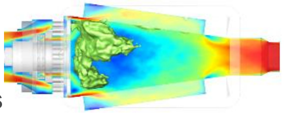


GPUs provide 10-15x speed-up over CPU

Ameen et al., DOE Advanced Engine Combustion Review Meeting, Aug 2021

CAPACITY AND CAPABILITY COMPUTING

INCREASING COMPUTATIONAL EXPENSE

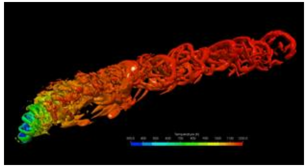


~0.1-0.5 mm grid size
O (10^3-10^4) processors

High-fidelity wall-resolved LES at limited conditions

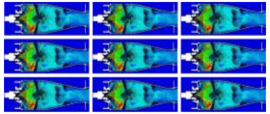
Subgrid models

CAPABILITY COMPUTING



~10 µm grid size
O (10^4-10^5) processors

DNS for generating gold-standard datasets at select conditions

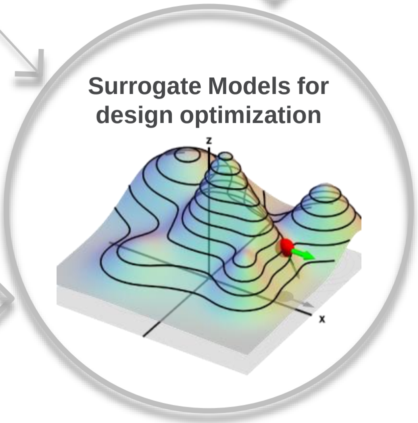


High-throughput design space exploration – RANS

Subgrid & wall models

CAPACITY COMPUTING

~0.5-1 mm grid size
O (100) processors



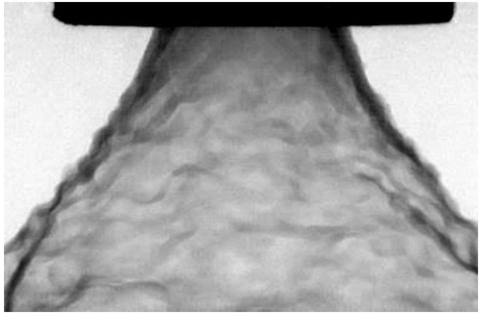
LEVERAGE A MULTI-FIDELITY SIMULATION FRAMEWORK

- Improve understanding of flow and combustion processes
- Develop physics-based and data-driven subgrid models
- Perform simulation-based design optimization
- Develop surrogate models for fast design optimization

X-RAYS: UNIQUE DIAGNOSTICS FOR MULTI-PHASE FLOWS

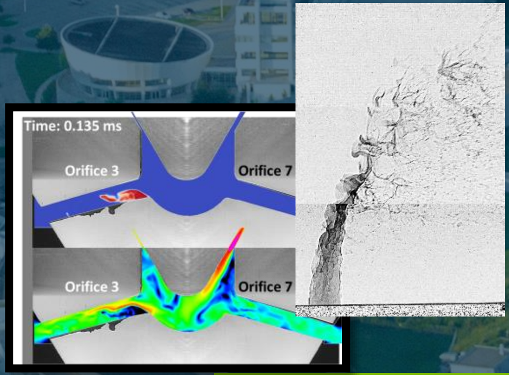
- Visible light is scattered by micron-scale droplets
  - Multiple scattering in regions of high droplet number density
  - Multi-phase flows are often opaque
- Small wavelength X-rays can penetrate multi-phase flows
  - Interaction is absorption of the x-rays by the fuel
  - Quantified to measure the **fuel density distribution, in dense regions of sprays**
- Synchrotron x-rays give **10^6 more flux than a benchtop source**
- **Excellent time, spatial resolution**

Radke (NASA), Meyer (Purdue)



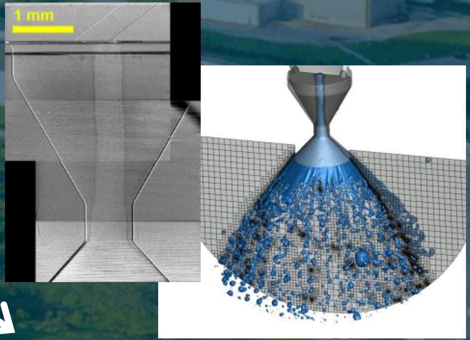
Radke (NASA), Meyer (Purdue)

PROPULSION AND POWER DEPARTMENT
UNIQUE DIAGNOSTICS AND HIGH-FIDELITY SIMULATIONS



DATA

- Advanced Photon Source
  X-ray Diagnostics
- RCM for fuels



KNOWLEDGE

- Internal Nozzle flow
- Atomization/ Fuel-air mixing
- Ignition
- Rare events: knock, misfire, flashback, lean blow-out
- Combustion stability
- SAFs, Advanced fuels (H_2, NH_3)

TOOLS

Super-computing resources
ML workflows

- Research: NEK5000, nekRS
- Design: CONVERGE, OpenFOAM, CharLES, …

Long history of technology transfer to industry via commercial tools

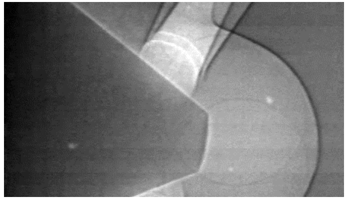
Argonne
NATIONAL LABORATORY

PISTON ENGINES: ON-ROAD, OFF-ROAD, RAIL, MARINE

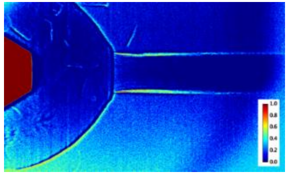
- X-RAY CHARACTERIZATION OF FUELS
- H2-ICE CHALLENGES AND OPPORTUNITIES
  - DNS of Internal combustion engine

X-RAY DIAGNOSTICS FOR LIQUID FUEL INJECTION

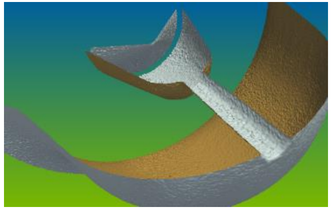
Needle Motion

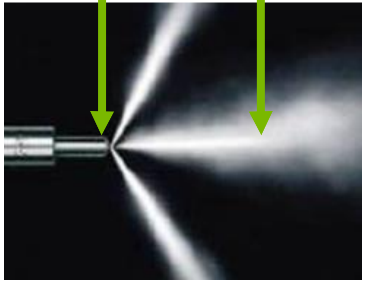


Nozzle Cavitation



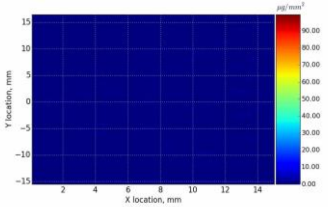
High Precision
Nozzle Geometry



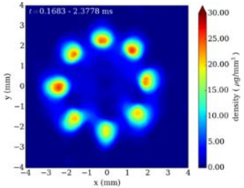


X-rays enable unique capabilities, both *inside* and *outside* the nozzle

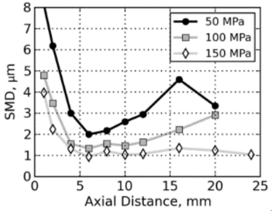
Near-Nozzle Fuel
Density



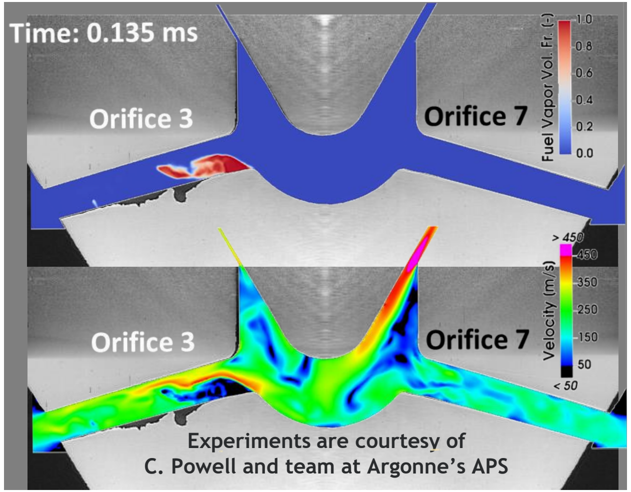
Spray Tomography

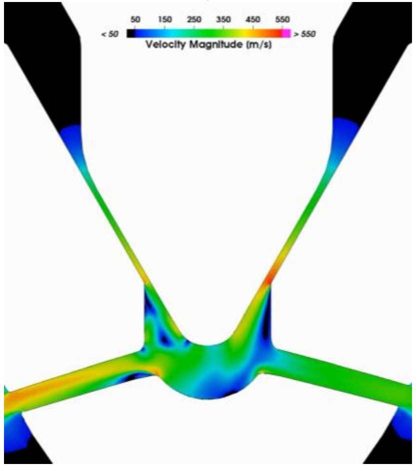


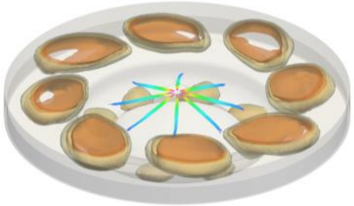
Spray Surface Area and SMD



X-RAYS TO SIMULATIONS

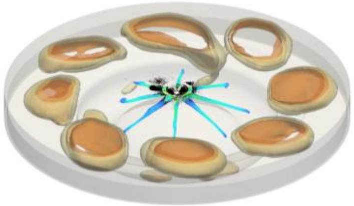




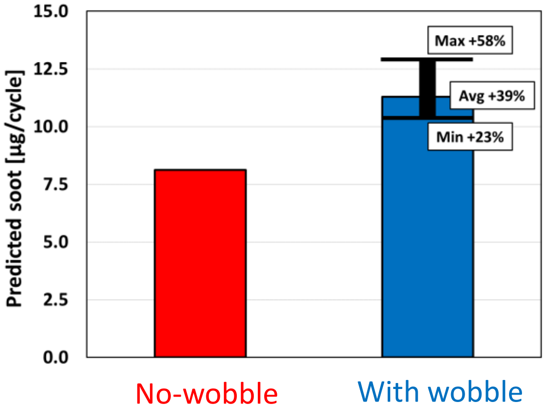


No-wobble

CONVERGENT SCIENCE

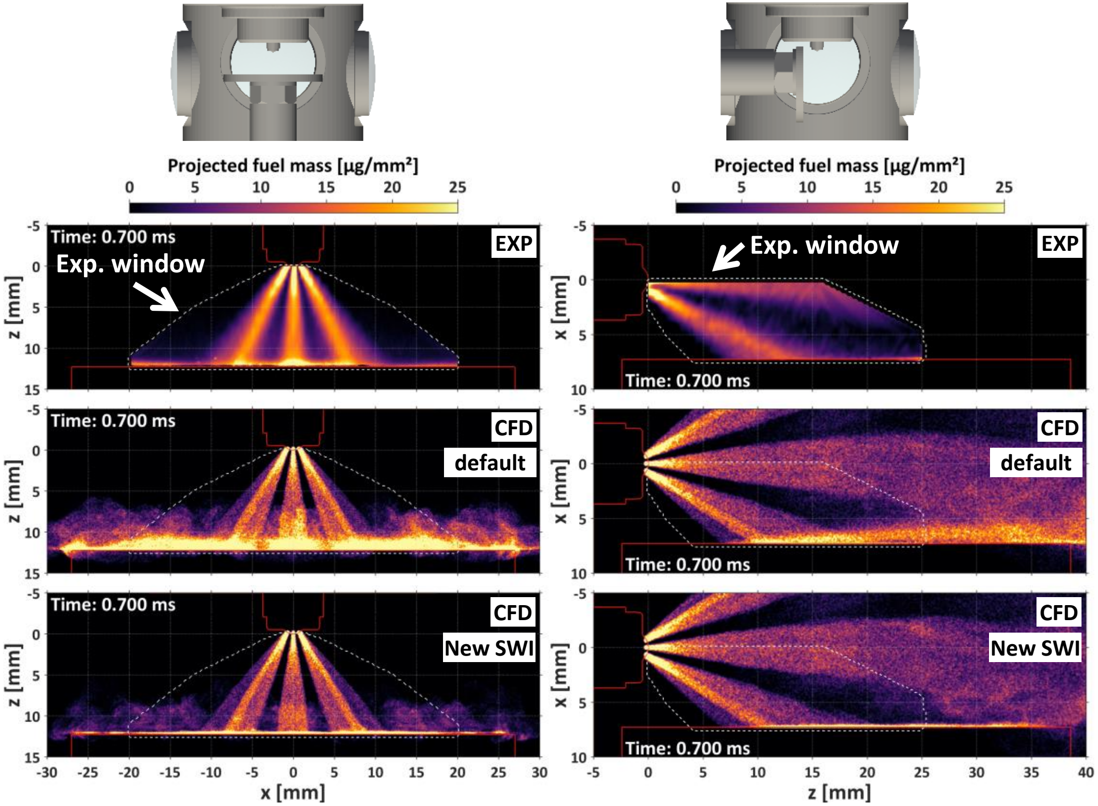


With wobble

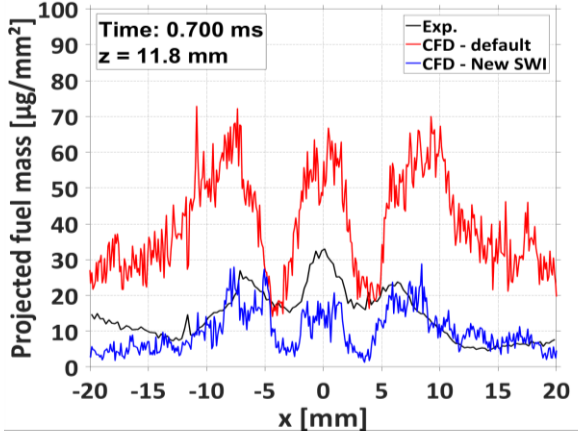


SPRAY-WALL INTERACTION (SWI)

Leveraging Unique X-ray Diagnostics

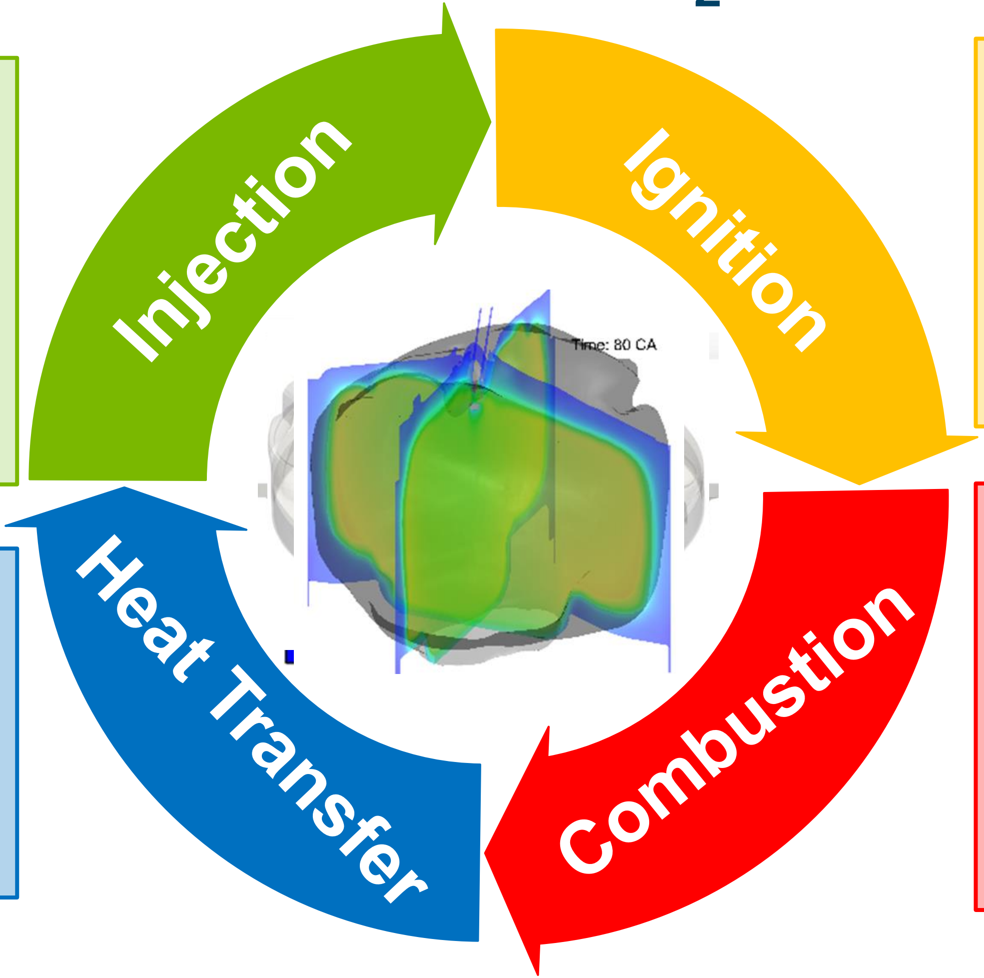


- Engine Combustion Network case (T=298 K, p=100 kPa)
- Higher fuel mass accumulation observed using default O'Rourke & Amsden model
- New SWI* model developed based on x-ray observations and DNS data from Prof. M. Raessi (U Mass.), incorporated in CONVERGE CFD code



* Torelli et al, *IJER*, 2020

KEY RESEARCH AREAS FOR H_2 ICE



Fuel Injection

- Gas-jet structure (mesh refinement, turbulence modeling, discretization order, timestep).
- Mixing with surrounding gas (mesh refinement, turbulence modeling, discretization order, mixing model).

Ignition

- Conventional SI (discharge, flame kernel growth).
- Advanced ignition (discharge, flame kernel growth, TCI).
- Diesel pilot (spray models, kinetics).

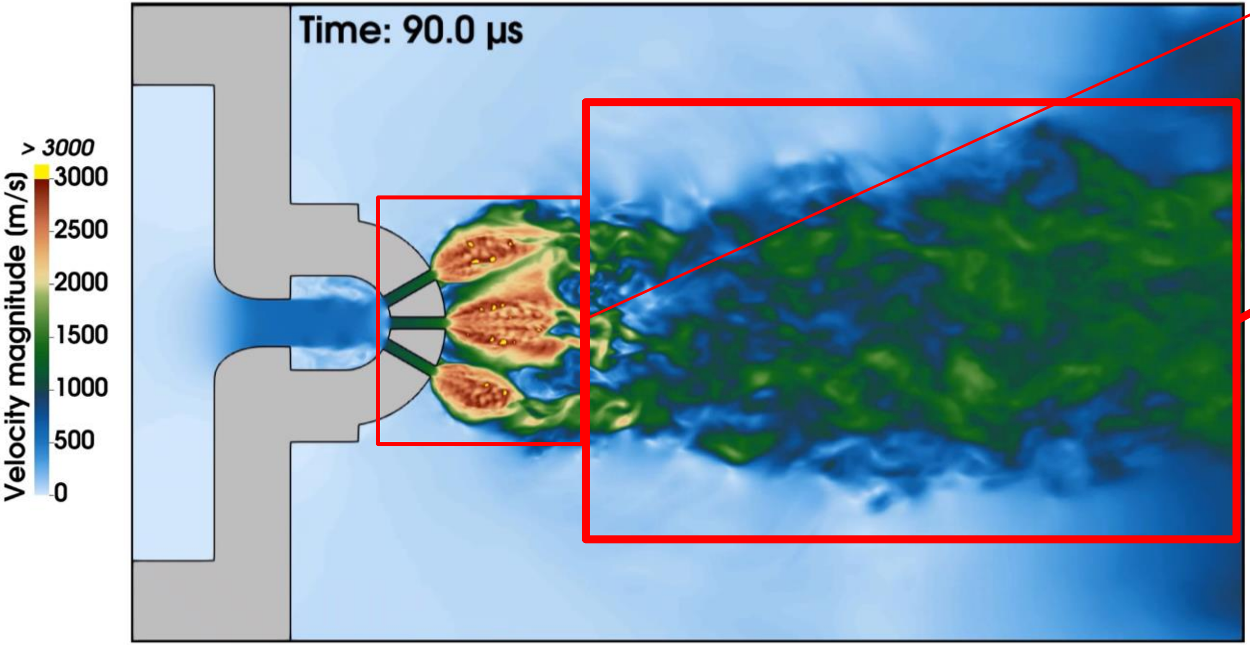
Combustion

- Flame speed (turbulent combustion modeling, kinetics, transport properties).
- Pre-ignition (CHT calculations, kinetics).
- Knock (CHT, knock modeling, kinetics).
- Emissions (kinetics).

Heat Transfer

- Wall temperature (CHT modeling).
- Wall heat fluxes (mesh refinement, turbulence modeling).
- Flame-wall interaction (quenching model).

HYDROGEN - DIRECT & PORT INJECTION



Focus Area 1

- Under-expanded (supersonic) gaseous jet region impacts jet evolution (eventually collapse) and determines the start of the mixing domain.

Focus Area 2

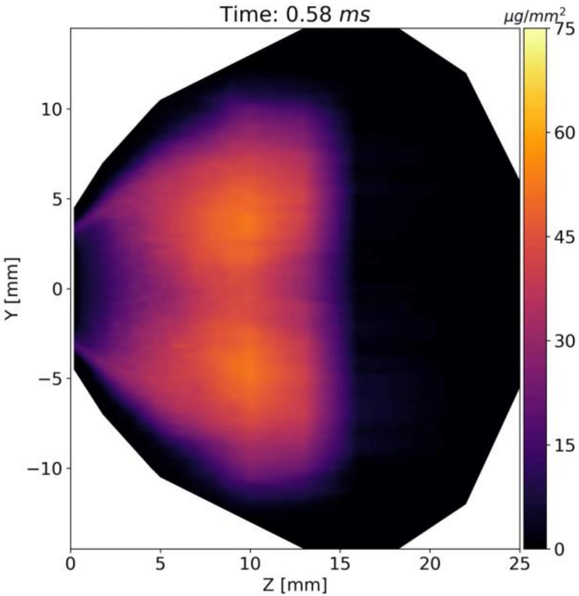
- Mixing between the injected gas and the ambient gas occurs throughout the gas-jet domain, starting from the jet boundaries into the jet core.

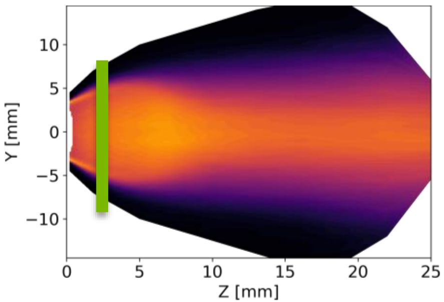
Additional Focus (Area 3) on the gas-jet impingement and interaction with cylinder walls.

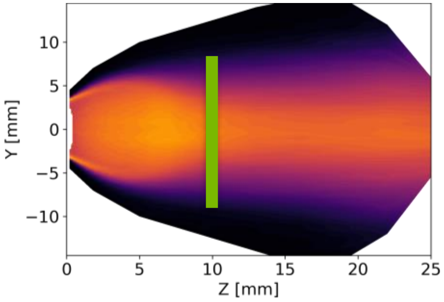
Port Fuel Injection (PFI) has similar challenges for Focus Areas 2 and 3

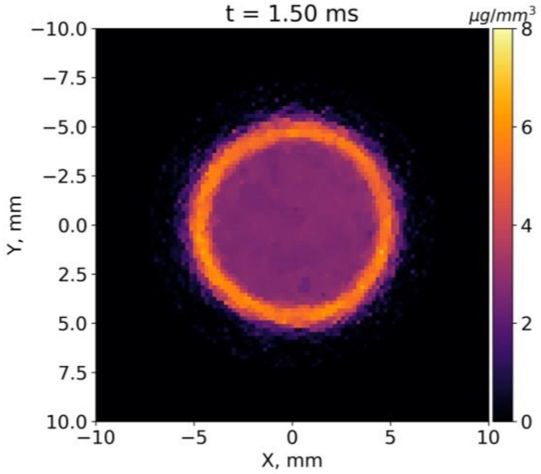
3D MEASUREMENTS OF GAS JETS WITH X-RAYS

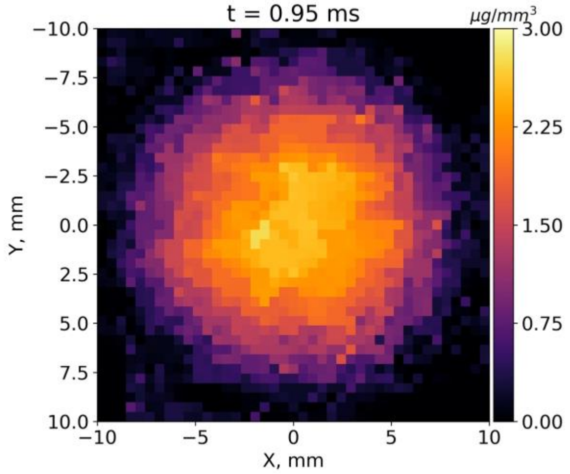
35 bar He /5 bar N_2







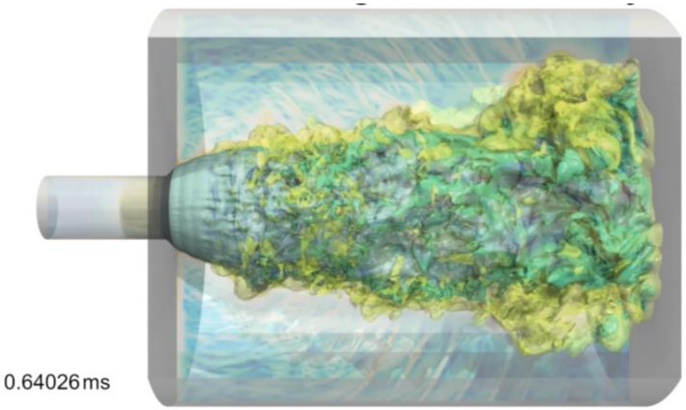




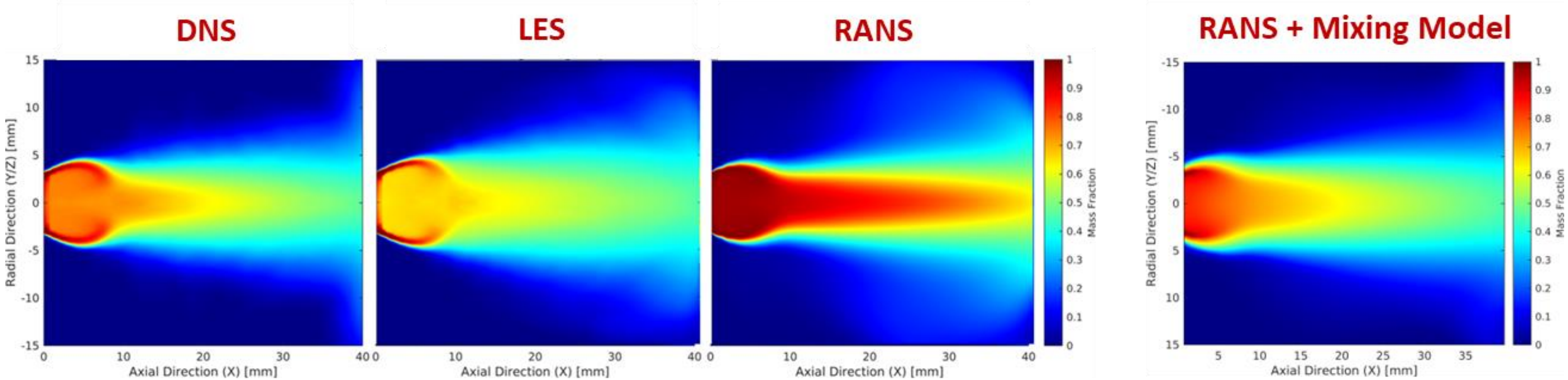
- He (and H_2) is transparent to x-rays and is a better surrogate than Argon
- X-ray CT allows measurement of the 3D density distribution for unique quantitative data of this collapse

MIXING MODEL DEVELOPMENT

- Mixing of H_2 under direct injection conditions remains a challenge
- DNS performed using compressible Nek for different Re conditions



	Hrs	Cores	Core-hrs
LES	59	540	31,860
RANS	19	180	3,420
RANS + mixing model	29	180	5,220

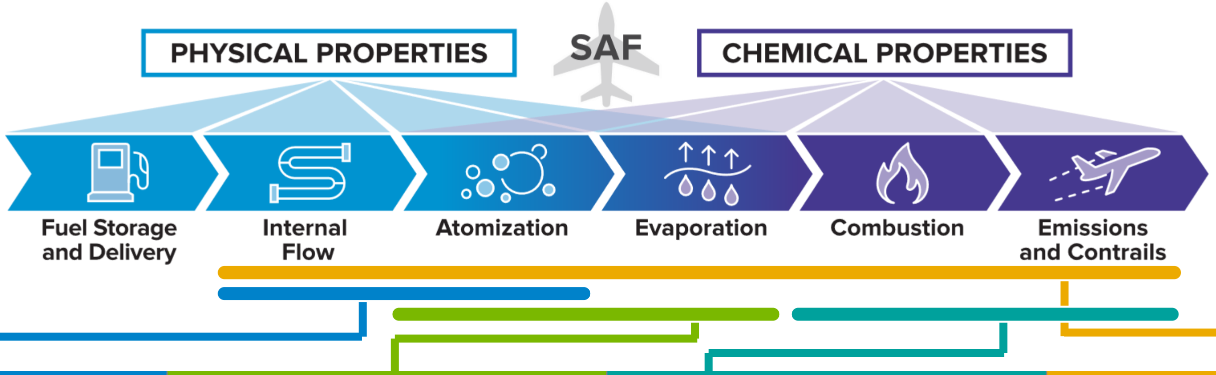


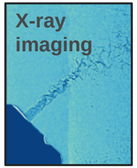
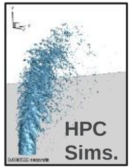
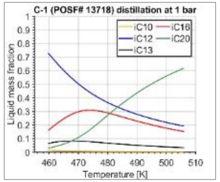
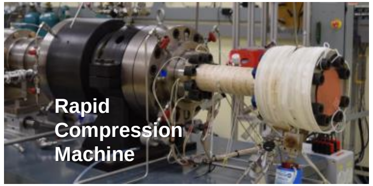
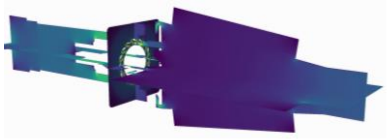
Azimuthal + Time Average Results

GAS TURBINES

- SUSTAINABLE AVIATION FUELS
- GAS TURBINE FILM COOLING

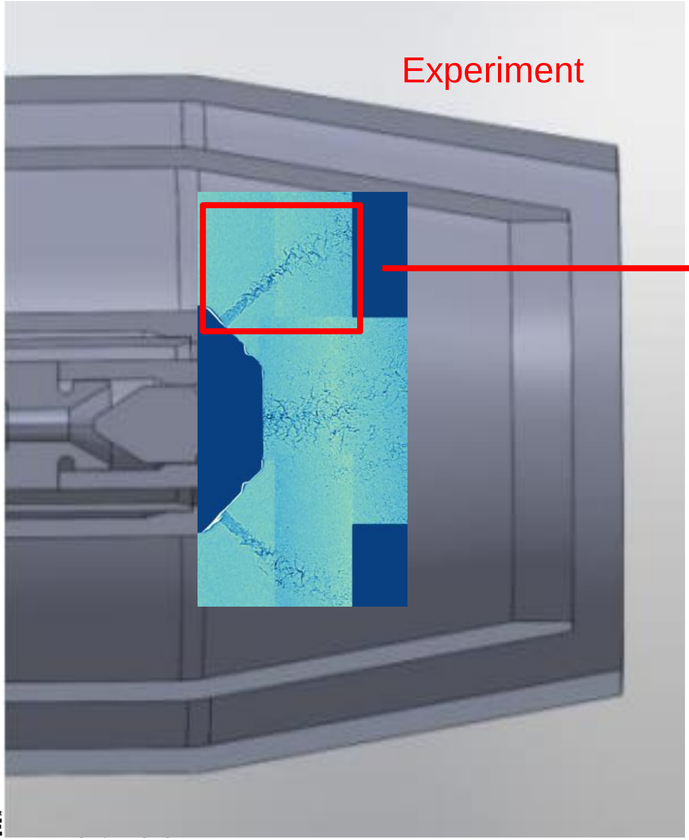
SYNTHETIC AVIATION FUEL: GAPS & OPPORTUNITIES

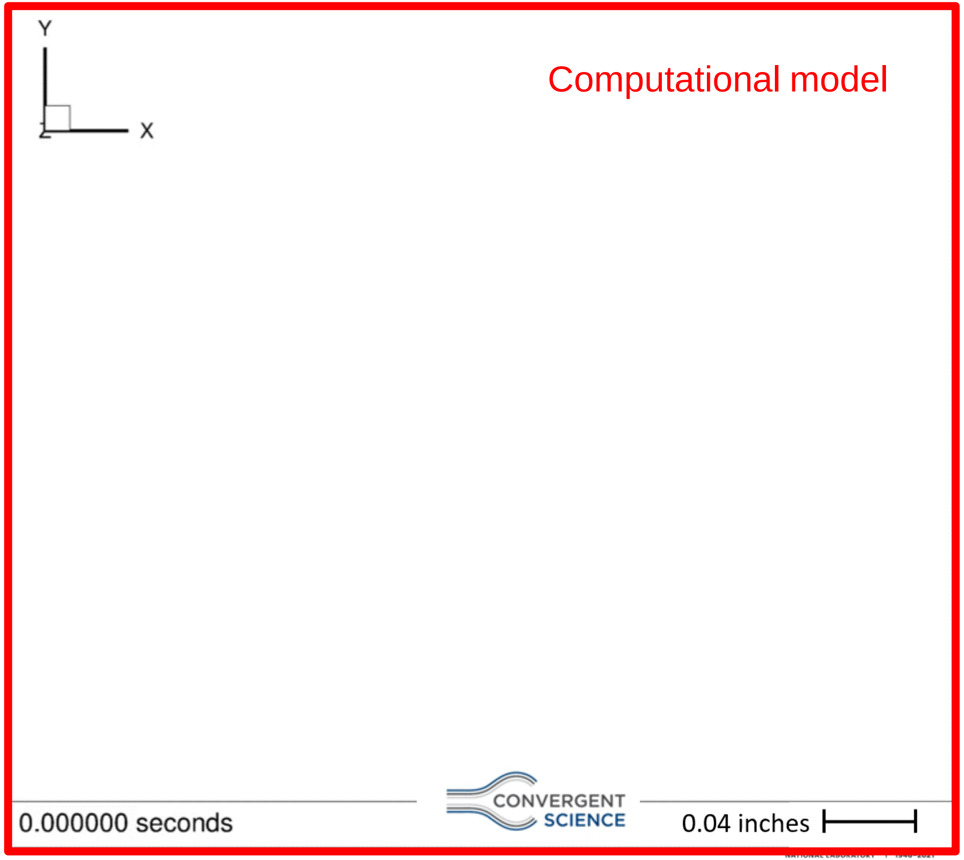


MULTIPHASE FLOWS	REAL FLUID BEHAVIOR	CHEMISTRY DYNAMICS	HIGH-FIDELITY COMBUSTION
 Non-proprietary atomizer  	SAF multi-component vaporization 		 Mid-size combustor CFD simulation
▪ Sprays primary influence downstream processes ▪ Resources (APS, ALCF) and expertise to impact OEM tools	▪ SAF chemistries influence physical processes ▪ Develop physics-based engineering models for multi-component vaporization	▪ Combustion, emission, contrail prediction hinge on SAF characterization ▪ Validating SAF models	▪ Gold-standard CFD to assess SAF ▪ Unifies multi-physics sub-models ▪ Uses ALCF, LCRC
▪ Lab/DOE investments in substantial facility upgrades ▪ Approach guided by OEMs to achieve impactful results	▪ Transferrable to industry practice	▪ Facility upgrades for wide range of SAF ▪ Coordinated with academia	▪ Predictive abilities; validation of engineering tools ▪ Assess critical FOMs and emissions/contrails

Fuels: A-2, C-1 -> HEFA-SPK, ATJ

JICF X-RAY EXPERIMENTS AND VOF SIMULATIONS

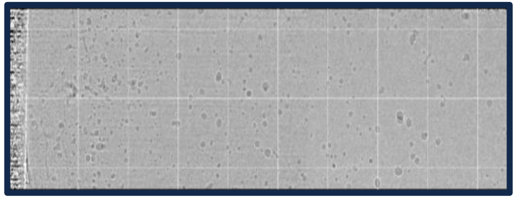




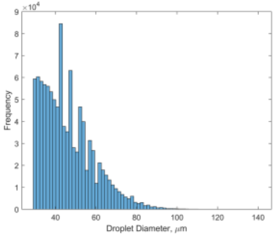
X-RAY SPRAY INPUTS FOR COMBUSTION SIMULATIONS

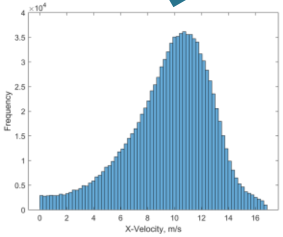
- X-rays provide initial spray conditions
- Prior work (in NJFCP) used downstream PDPA measurements to initialize sprays

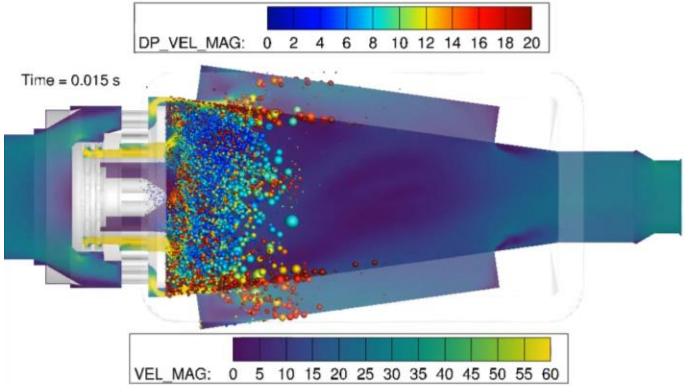
X-Ray near nozzle imaging

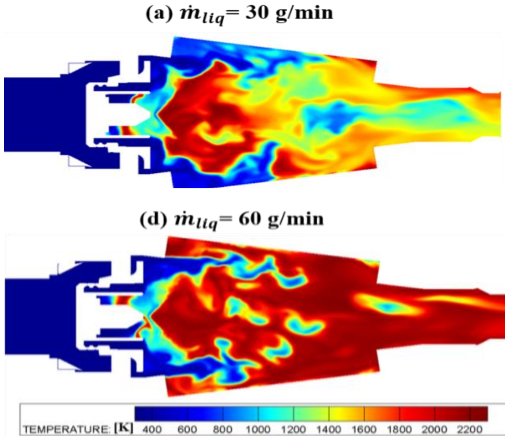


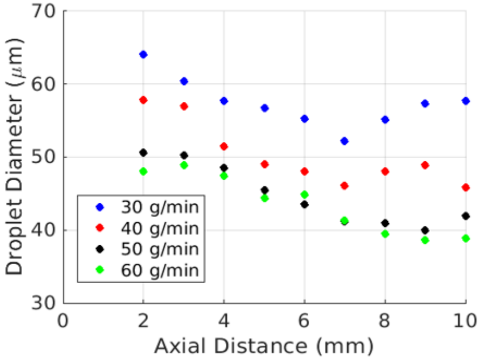
Spray Boundary Conditions









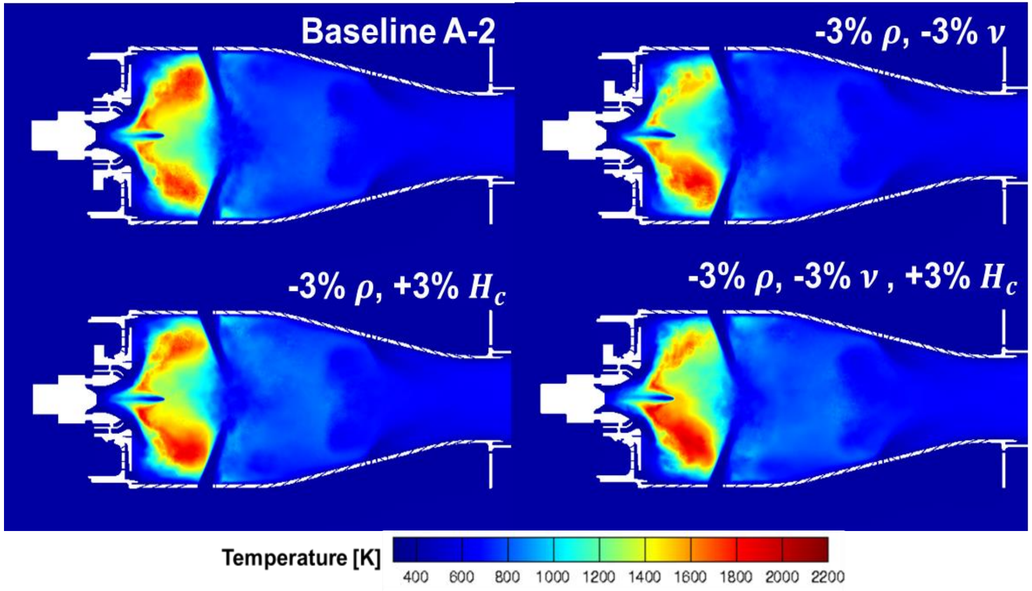


* Dasgupta et al., 2022 AIAA SciTech Forum

Collaboration: C.B Kweon, J. Temme, E. Mayhew (ARL), Experimental data – Prof. Tonghun Lee & team (UIUC)

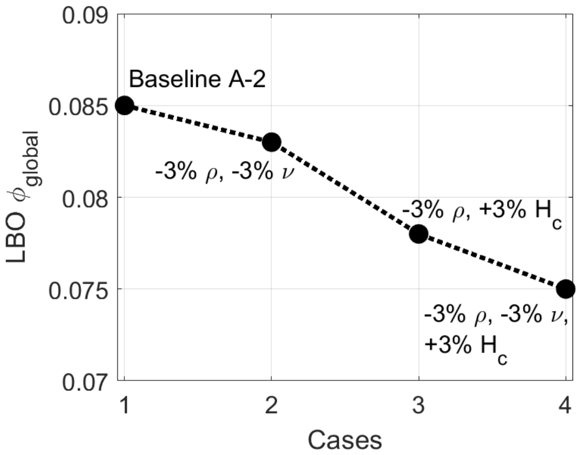
ARE SAF FULLY "DROP-IN"?

NJFCP Referee Rig simulations



	Density (ρ) @ 15ºC	Kinematic Viscosity (ν) @ -20ºC	Heat of Combustion (H_c)
A-2	803 kg/m^3	4.5 cSt	43.1 MJ/kg

- Fuel property changes are within ASTM limits for being drop-in!
- Small changes lead to changes in temperature and species distributions resulting in heat release changes and lean blow out limits



Dasgupta et al., ASME Turbo Expo 2024

ML-BASED SUB-GRID SCALE MODEL FOR GAS TURBINE FILM COOLING

Motivation: ***Bridge the gap***

Wall-Resolved LES (WRLES)

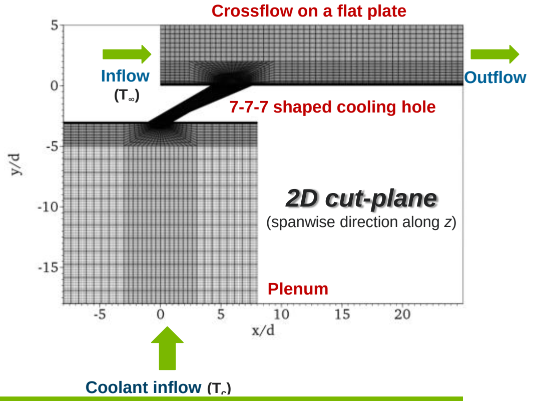
Pro: High accuracy

Con: High cost (fine near-wall resolution)

Wall-Modeled LES (WMLES)

Pro: Lower cost (coarse near-wall resolution)

Con: ~~Low accuracy~~



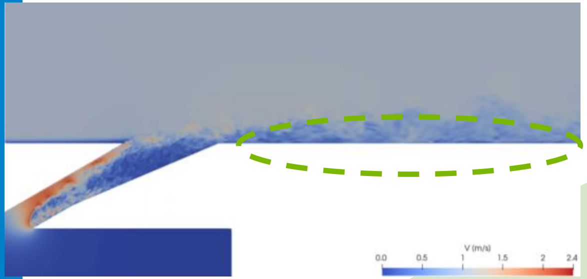
Use 3D high-fidelity WRLES data for training

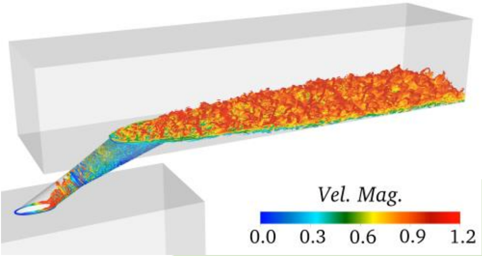
Data-driven subgrid model for wall shear stress

Deploy data-driven wall model in coarse WMLES

DATA-DRIVEN WALL MODEL DEVELOPMENT

RTRC
Raytheon Technologies Research Center





High-fidelity WRLES for different blowing ratios, hole angle using Nek5000

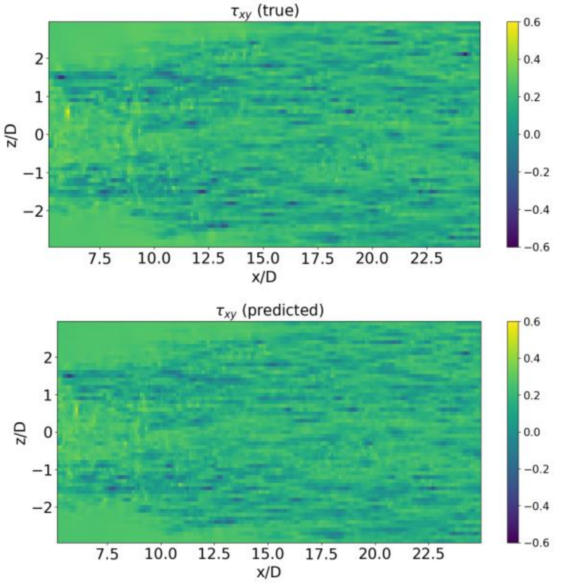
Data post-processing to extract flow datasets for ML training

$u_i, \frac{\partial u_j}{\partial x_i}, \frac{\mathrm{d}p}{\mathrm{d}x_i}, \rho, \mu, \tau_{xy}$, etc.

Hyperparameter optimization

CUDA for GPU training

***A priori* & *A posteriori* validation**



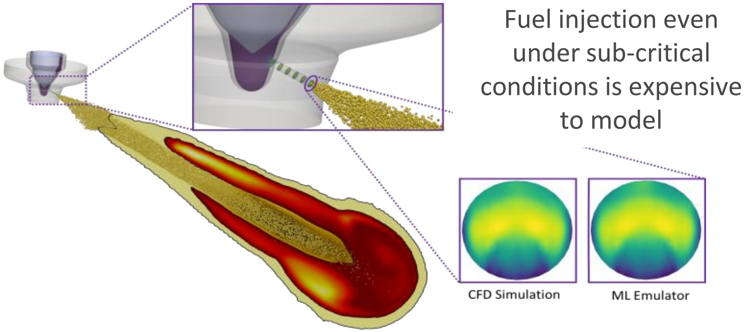
HPC4 ENERGY INNOVATION

Nunno et al.
AIAA SciTech 2022-1404

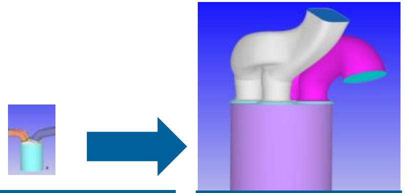
Kumar et al.
AIAA SciTech 2023-1254

CONCLUDING REMARKS

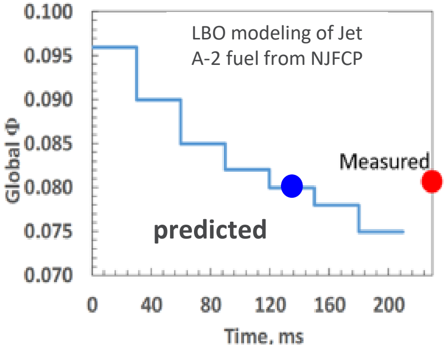
- Ability to rapidly predict and understand causalities of rare events, e.g., engine knock, pre-ignition, flashback, lean blowout, etc.
  - Long time-scale problem with large run times
  - Persistent across all combustion domains, especially with alternate fuels
- Sub-critical, trans-critical and supercritical transition for fuel injection and multi-regime combustion.
- Conjugate heat transfer and effect of fuels
- ECP funded codes have capability for DNS like calcs using hybrid architectures. Lot of ground-truth data developed but have not been mined for ROMs.
- Can foundational models for combustion help?
- Technology transfer to industry to accelerate pace of innovation!



Fuel injection even under sub-critical conditions is expensive to model



8.6 cm bore 9.5 cm stroke 16.6 cm connecting rod	25 cm bore 32 cm stroke 59 cm connecting rod



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  - DOE, FECM: Robert Schrecengost, John Crane
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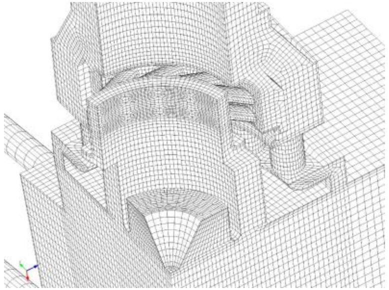
  - Laboratory Computing Resource Center, Argonne Leadership Computing Facility
  - Advanced Photon Source, Argonne
  - 2021 INCITE Computing Award, Several ALCC awards

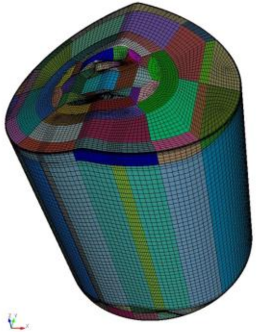
THANK YOU!

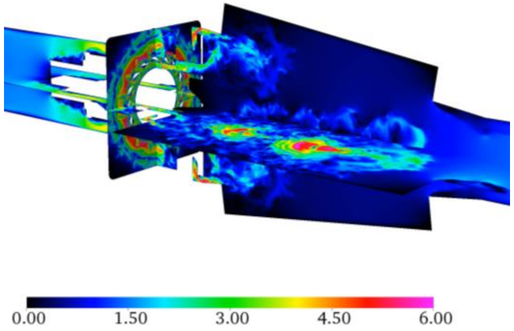
GOLD-STANDARD DNS/LES

Nek5000/NekRS: Exascale CFD Code

- Spectral element method (SEM):
  - Solution represented as N^{th} order tensor-product polynomials (N~ 5-15)
  - Exponential (spectral) convergence with N
- Semi-implicit and characteristic-based temporal schemes (up to 3rd order accurate)
- Supports fully unstructured hexahedral meshes generated using 3rd party softwares (Pointwise, Cubit)
- NekRS - GPU variant of Nek5000:
  - GPU-ready exascale code
  - Successfully deployed on Polaris, Frontier, and Aurora
- Nek5000 (CPU version) can also handle Lagrangian sprays and fully compressible flows (shocks, detonations)
- Other features: CHT, moving/deforming meshes, overlapping grids, LES/RANS turbulence models
- Ideal for **<u>gold-standard DNS/LES</u>** for complex flow problems and develop/improve **<u>physics-based and ML-based models</u>**



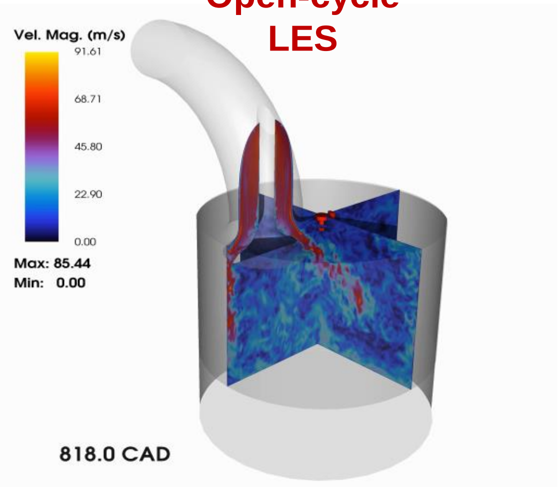




DNS > 350M grid points

DNS OF ICE FLOWS WITH Nek5000

Open-cycle LES

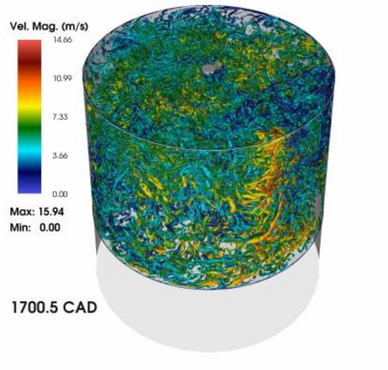


LES – Fuel Injection

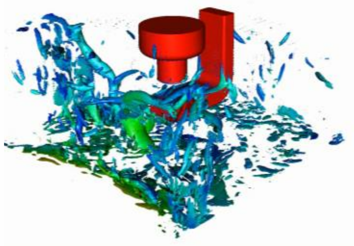
Multi-cycle LES showed good agreement with PIV. Flow-field used to investigate causes of CCV.

- LES > 95M grid points, scales on >16K procs
- DNS > 430M grid points, scales on >51K procs

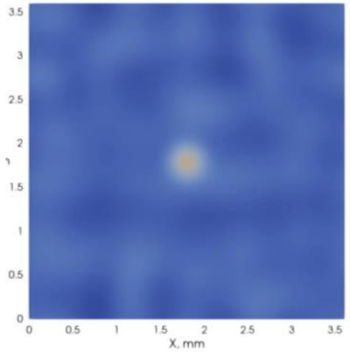
Closed-cycle DNS



DNS near-spark plug



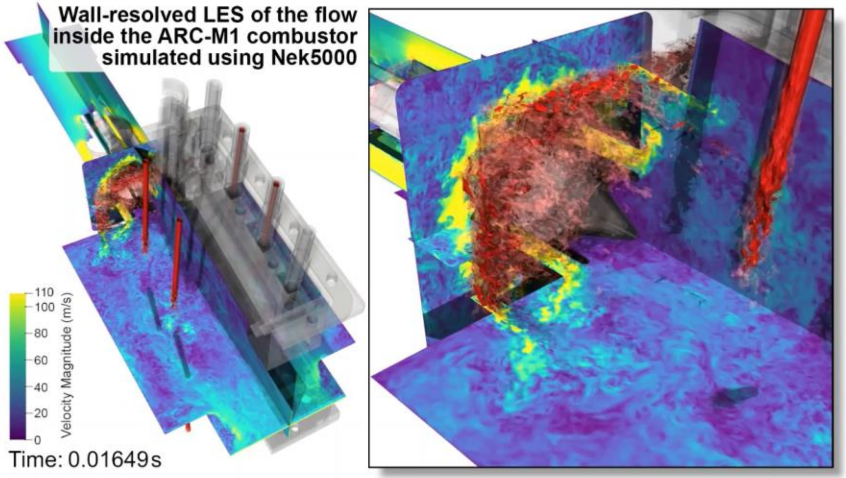
DNS – SACI Combustion



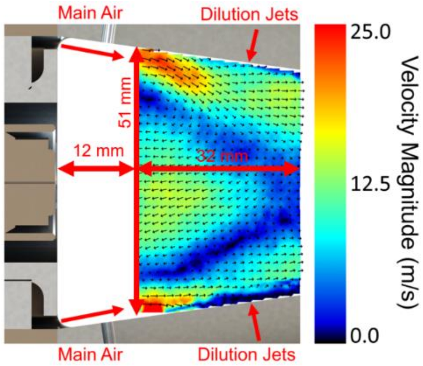
- Developed improved heat transfer, ignition, and combustion models for industry use

* https://www.energy.gov/eere/vehicles/downloads/direct-numerical-simulation-dns-and-high-fidelity-large-eddy-simulation-les

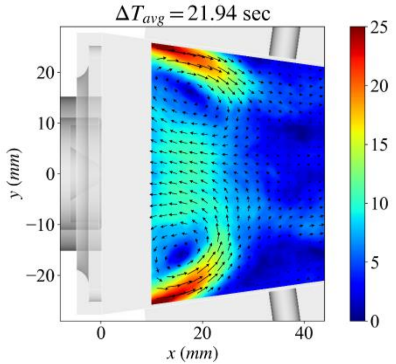
WALL-RESOLVED LES OF GAS TURBINE FLOWS



Validation of Flow-field Statistics



PIV



LES

Simulation parameters	
Polynomial order	7
Element count	1.1M
Number of grid points	580M
Max/Min Δx	0.52/0.005 mm
Reynolds number	58,200
Wall time/FTT	24 hrs (256 nodes on Theta)

- Wall-resolved LES of the flow inside the ARC-M1 combustor performed using Nek5000*
- Simulations provided key insights into the turbulent flow structures, recirculation zones, and flow interactions between main and dilution flows
- POD analysis was performed to investigate turbulent flow structures

*Simulations have also been repeated with NekRS on OLCF Frontier

[1] Wu, Dasgupta, Ameen, Patel (2023) AIAA SciTech

SURROGATE MODELING OF THE IMPACT OF MANUFACTURING UNCERTAINTIES ON GAS TURBINE FILM COOLING EFFICIENCY

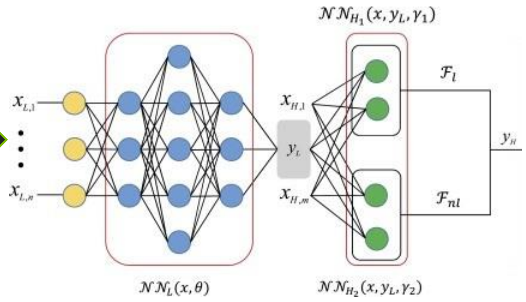
Multi-fidelity deep learning to predict the effect of in-hole surface roughness on film cooling effectiveness

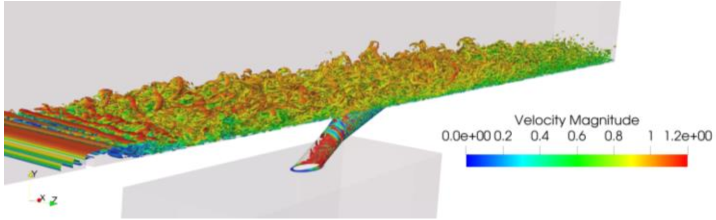
Wall-resolved LES (WRLES)
High accuracy, high cost

Wall-modeled LES (WMLES)
Medium accuracy, medium cost

Unsteady RANS
Low accuracy, low cost

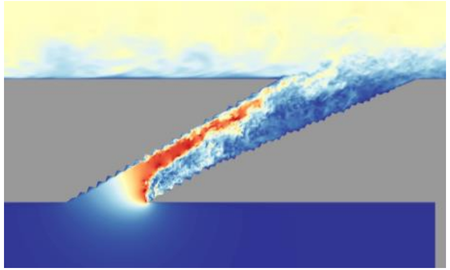
Multi-fidelity simulation dataset





Composite NN surrogate model to quantify surface roughness effects

Hierarchy of CFD model fidelities in NekRS



Rough cooling hole

DOE-AMMTO

HPC4 ENERGY INNOVATION

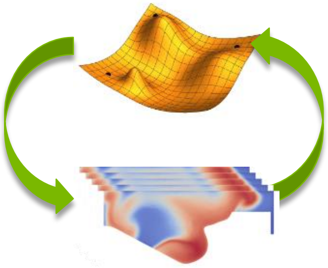
Jarrah et al.
AIAA Aviation 2024-1404

RTRC Raytheon Technologies Research Center

Argonne NATIONAL LABORATORY 75 1946–2021

TECHNOLOGY TRANSFER TO INDUSTRY

AI based optimization tools and x-ray data transferred to software vendors



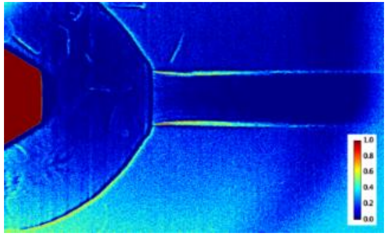
Parallel Works

CONVERGENT SCIENCE

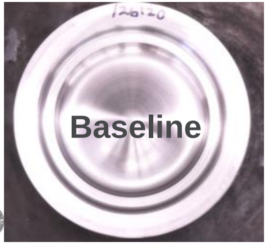
R&D 100 AWARDS 60TH ANNIVERSARY 2022

Argonne's data and tools are integrated into Cummins's Analysis Lead Design process for design of fuel injector and combustion systems

Cummins



Improved efficiency and reduced soot by designing new pistons & injection strategies



CAT

Assisted Progress Rail improve efficiency and meet Tier – 4 compliance with single cylinder engine research

Progress Rail

A Caterpillar Company