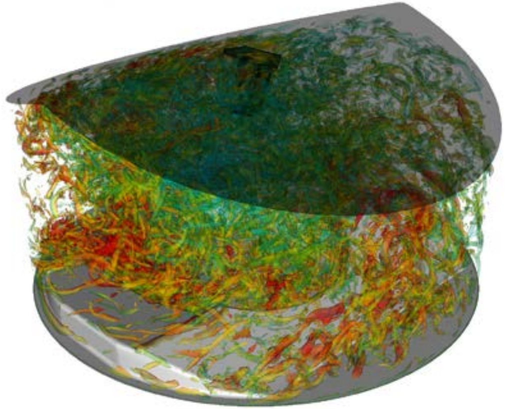
REIMAGINING IC ENGINE DEVELOPMENT LEVERAGING NEXT-GENERATION HPC & AI



SIBENDU SOM
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Co-chair, US DRIVE Advanced Combustion and Emissions Control (ACEC) Tech Team

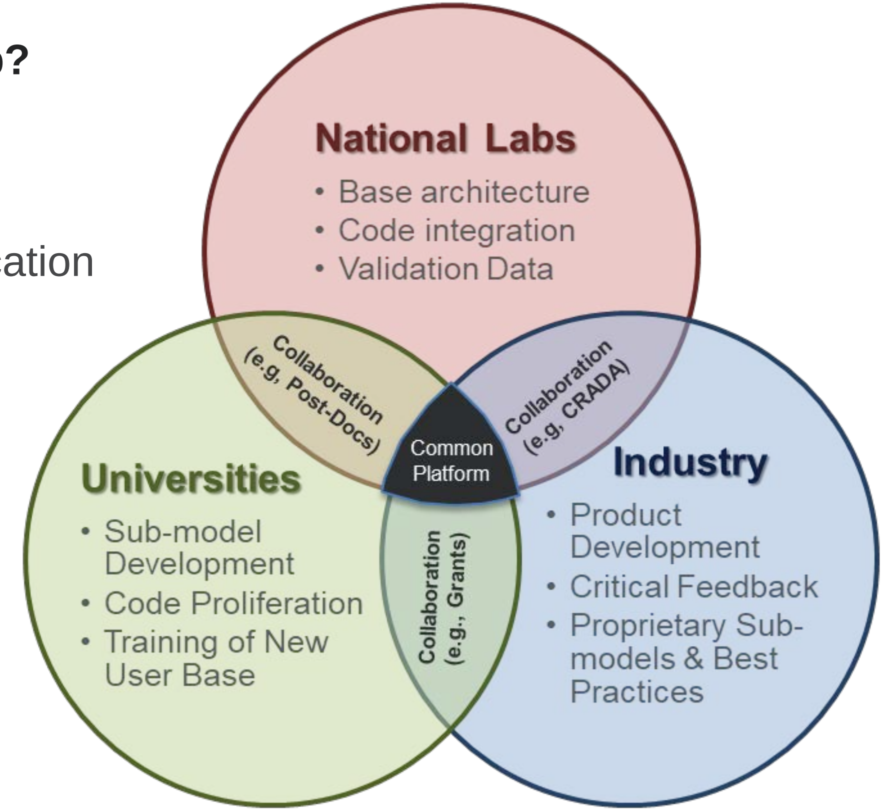
MODELING ECOSYSTEM THEN …

What was the common working relationship?

1. Centered around a common code platform
2. Each entity had particular strengths
3. Strong user community and open communication

Why did this working model change?

1. Complexity of proprietary combustion systems (meshing/sub-models)
2. Need for stronger parallelization (flow/chemistry)
3. User support & code maintenance
4. Growth and emergence of commercial codes



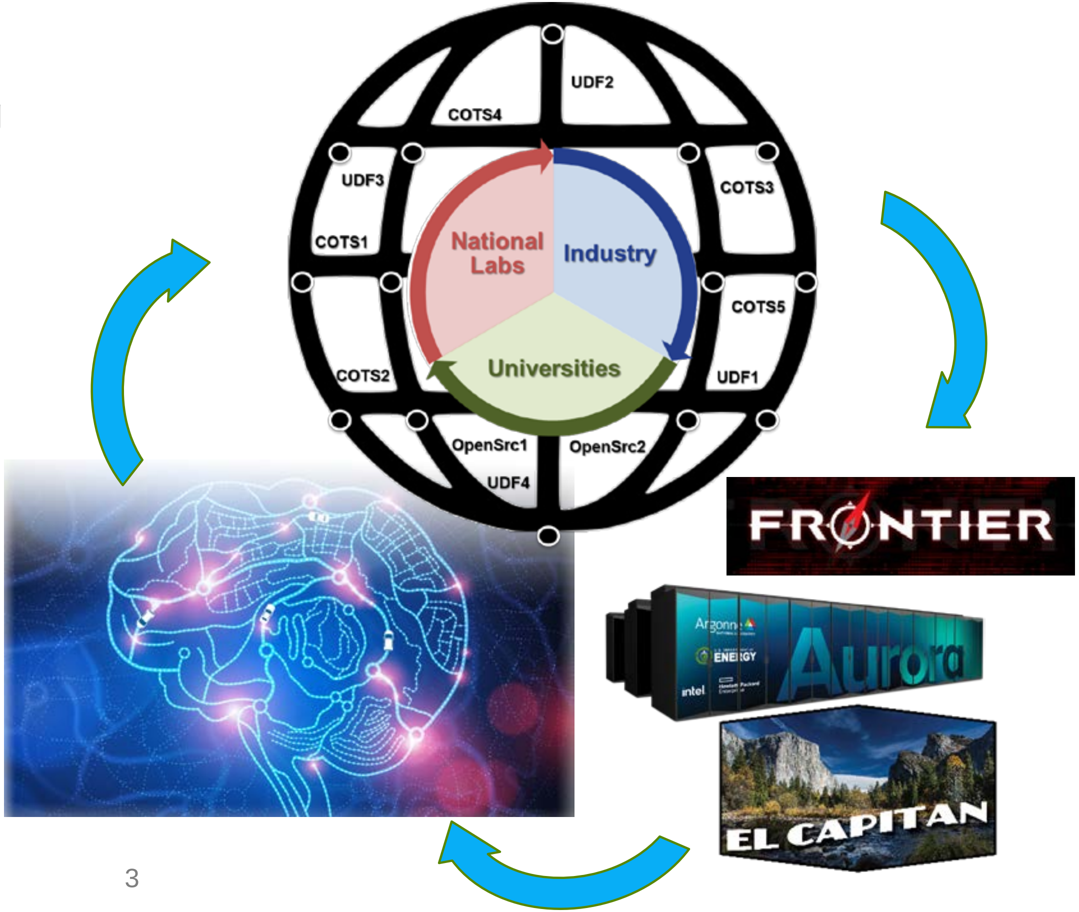
MODELING ECOSYSTEM NOW …

1. Institutions centered around a growing ‘web’ of commercial (COTS) and open source options

2. Implementing UDFs into commercial codes with need for validation

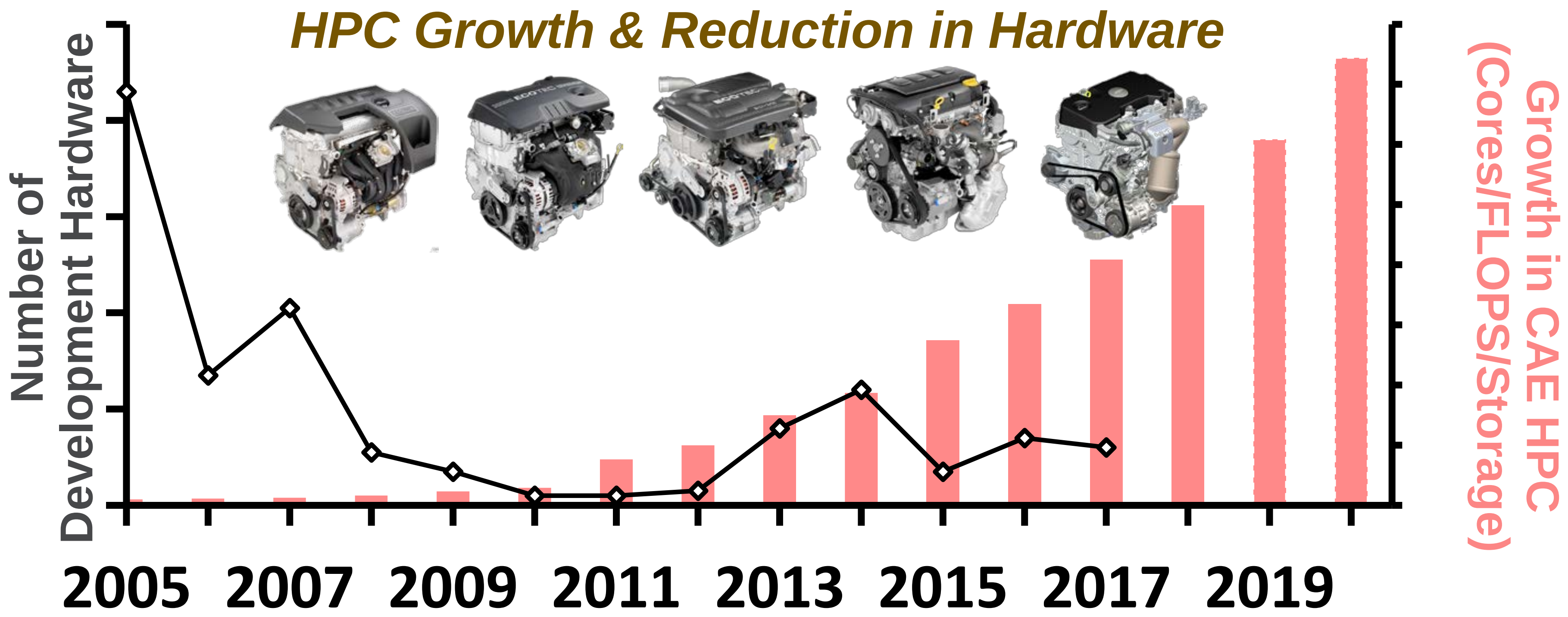
3. Heavy investment in national laboratory supercomputing infrastructure (drive to exascale)

4. Opportunities to accelerate machine learning and artificial intelligence



CAE IS VITAL FOR FUTURE PROPULSION SYSTEMS

<u>Goal</u>: First time capable designs to reduce iterations in the physical world



ASME ICEF Panel, 2019

INCREASED DEMAND FOR FAST, VALIDATED MODELS

1. Design direction
   – Directional accuracy is important

2. Meet requirements or not
   – Accuracy is important (not much room for error)

3. Hardware out of the loop
   – Accuracy is important (not much room for error)

*Can we do it **faster**? Can we do it **cheaper**? Can we do something **new**?*

DOE HPC ROADMAP LEADS TO MULTIPLE EXASCALE SYSTEMS

FY 2012 › FY 2016 › FY 2018 › FY 2021 › FY 2022 › FY 2023

FY 2012

TITAN*
ORNL
Cray/AMD/NVIDIA

MIRA*
ANL
IBM BG/Q

SEQUOIA*
LLNL
IBM BG/Q

*decommissioned

FY 2016

THETA
ANL
Cray/Intel KNL

CORI
LBNL
Cray/Intel Xeon/KNL

TRINITY
LANL/SNL
Cray/Intel Xeon/KNL

FY 2018

SUMMIT
ORNL
IBM/NVIDIA

SIERRA
LLNL
IBM/NVIDIA

FY 2021

PERLMUTTER
LBNL
HPE/AMD/NVIDIA

FRONTIER
ORNL
HPE/AMD

FY 2022

AURORA
ANL
HPE/Intel

CROSSROADS
LANL/SNL
HPE/Intel

FY 2023

EL CAPITAN
LLNL
HPE/AMD

EXASCALE SYSTEMS

FOUR PRIMARY ALLOCATION PROGRAMS

For access to DOE Leadership Computing Facilities (OLCF and ALCF)

10% Director's Discretionary

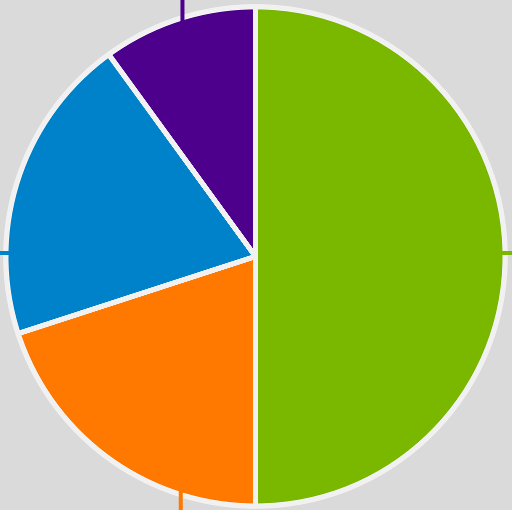
OAK RIDGE National Laboratory — Argonne NATIONAL LABORATORY

UP TO 20% ECP

Exascale Computing Project

20% ALCC

ASCR Leadership Computing Challenge



50% U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

OAK RIDGE National Laboratory — Argonne NATIONAL LABORATORY

TOWARDS PREDICTIVE ENGINE SIMULATIONS

EXPERIMENTS
Optical & Metal engines, RCM, APS, ...

Design new experiments / condition

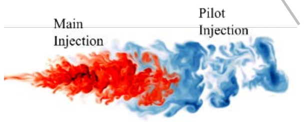
Validation

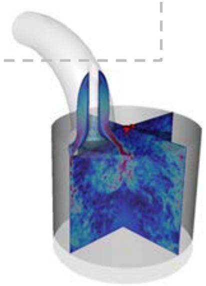
PELE
DNS of engine condition

Initial & Boundary conditions

NEK5000
DNS & LES of PACE engines

SOFTWARE TECHNOLOGIES
Math libraries, Co-design, …





- Gold-standard data for AI => unearth new physics
- Fast solvers
- Physics based & data driven models for:
  - Ignition
  - Sprays
  - Turbulent combustion
  - Kinetic mechanisms

Feedback

COMMERCIAL CFD TOOLS

- Scales on exascale architecture
- PACE models
- Used by industry

USCAR TECH TEAMS & OEMS

Emphasis with Nek and commercial codes for hybrid computing architectures

PACE leads: M. Weismiller (DOE), M. McNenly (LLNL), S. Som (ANL), J. Szybist (ORNL), P. Miles (SNL)

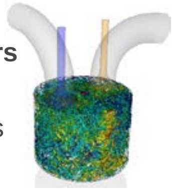
VISION
MULTI-FIDELITY SIMULATION FRAMEWORK

INCREASING COMPUTATIONAL EXPENSE

CAPABILITY COMPUTING

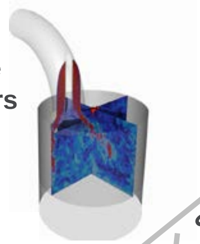
~10 μm grid size
O (10^4-10^5) processors

DNS for generating gold-standard datasets at select conditions

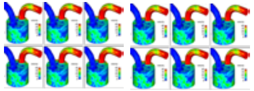


~0.1-0.5 mm grid size
O (10^3-10^4) processors

High-fidelity wall-resolved LES at limited conditions



Subgrid models



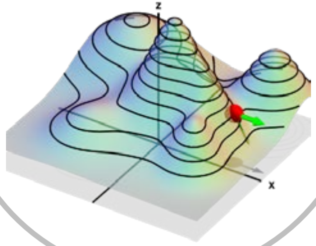
High-throughput design space exploration – RANS

Subgrid & wall models

CAPACITY COMPUTING

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

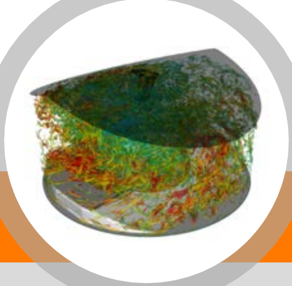
Surrogate Models for design optimization



LEVERAGE A MULTI-FIDELITY SIMULATION FRAMEWORK TO:

- 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

EXISTING EFFORTS IN HPC & AI



HPC

HPC used as a microscope – illuminating processes that are inaccessible to experimentation

HPC simulations provide a benchmark for accuracy of engineering simulations

AI

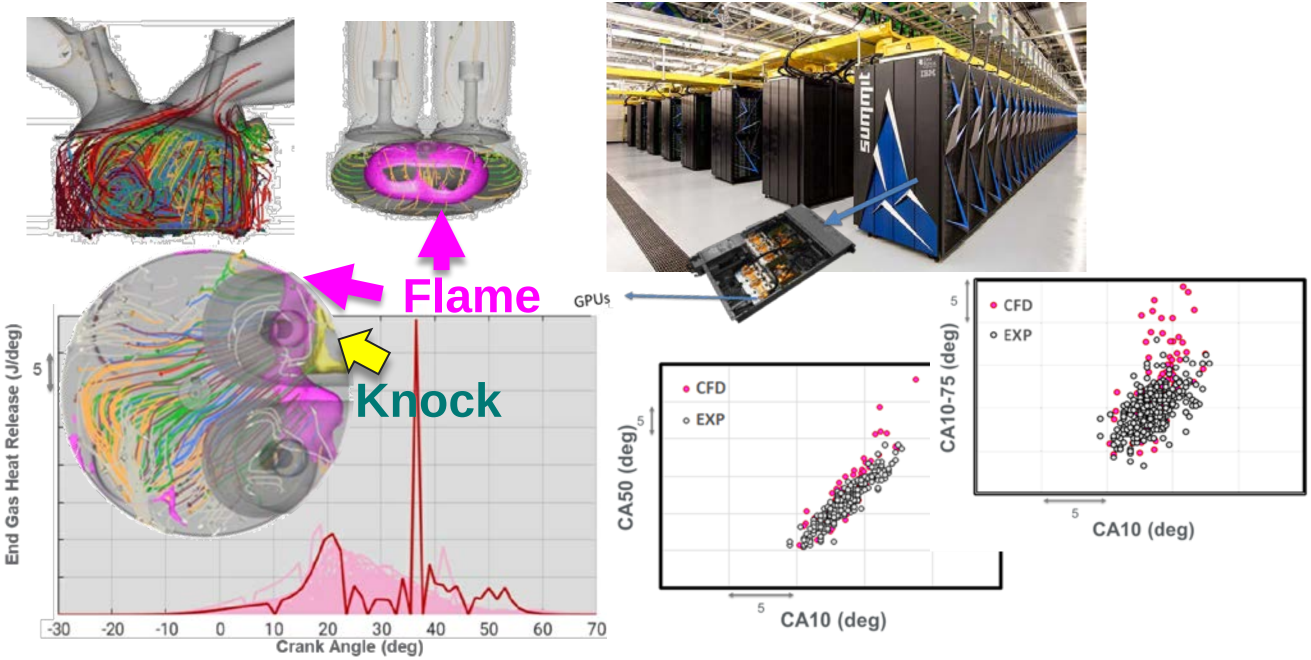
Machine learning and pattern recognition will be applied to

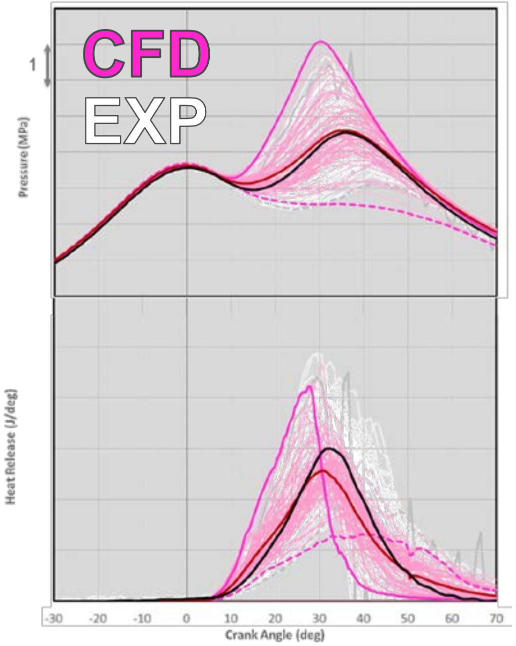
- Resolve decades-old problems (e.g. root causes of cyclic variability)
- Accelerate CFD simulations
- Develop reduced order models enabling optimal CFD-based design
- Develop data-driven, accurate and efficient sub-models

PACE leads: M. Weismiller (DOE), M. McNenly (LLNL), S. Som (ANL), J. Szybist (ORNL), P. Miles (SNL)

EXAMPLE OF CAPACITY COMPUTING

- Direct computation of combustion metrics over several computed engine cycles
- Fuel surrogate development matching chemical and physical properties
- Combined flame propagation (G-eqn), detailed kinetics simulations, and dynamic meshing
- National laboratory supercomputing leveraging GPUs (Zero-RK solver)



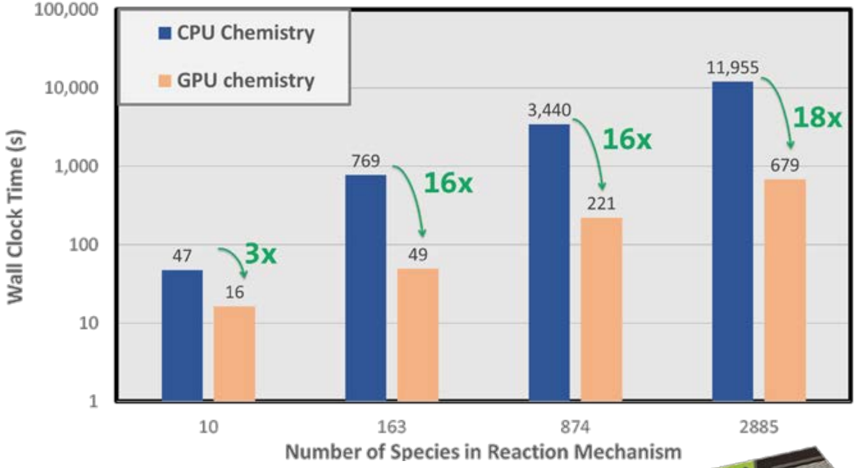


LES4ECE, 2021

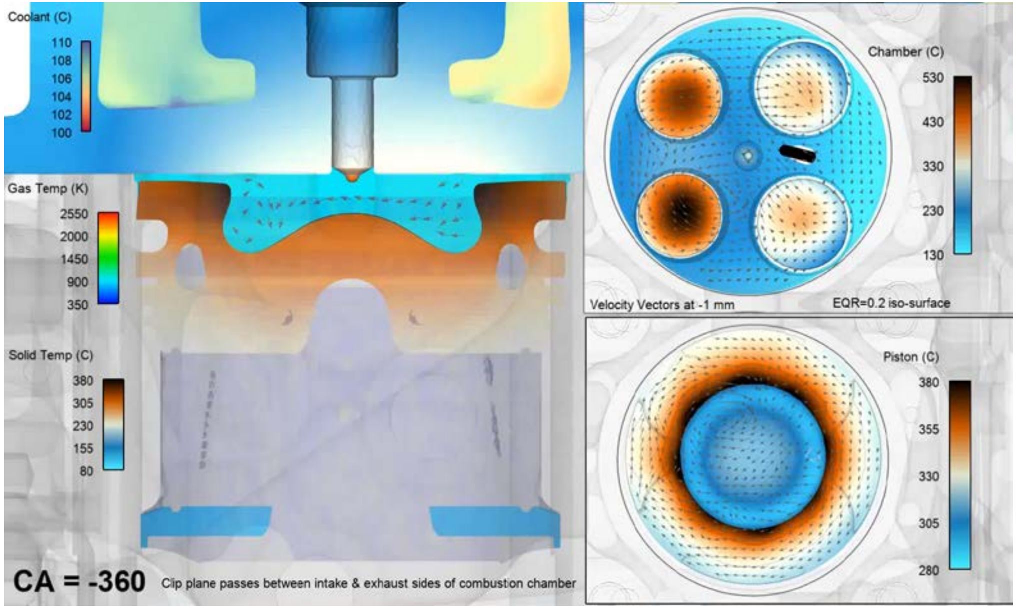
EXAMPLE OF CAPABILITY COMPUTING

gm | OAK RIDGE National Laboratory | Lawrence Livermore National Laboratory | OLCF Oak Ridge Leadership Computing Facility

GPU chemistry allows use of highly detailed reaction mechanisms



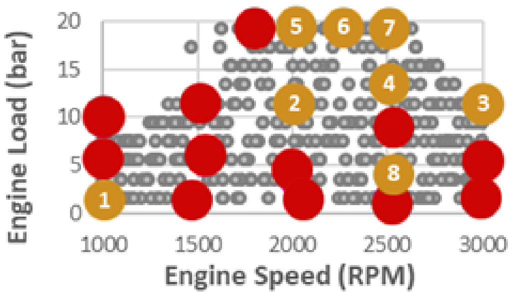
Fully coupled 3D CHT modeling for accurate wall temperature distributions



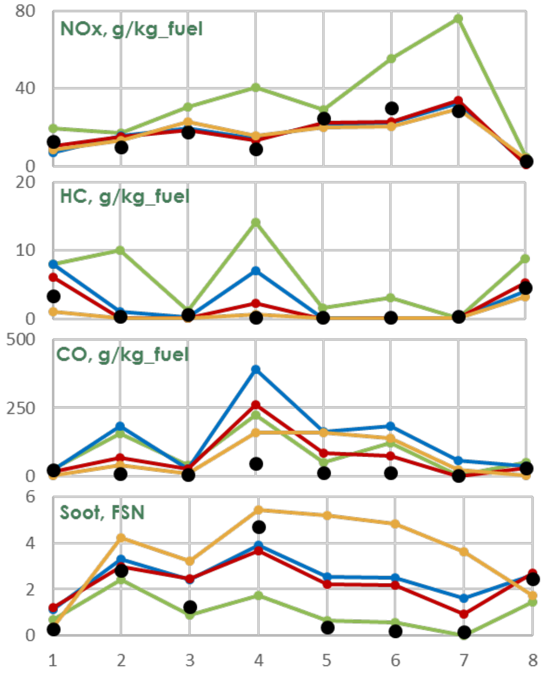
ASME ICEF Panel, 2019

COMPARISON OF EMISSION PREDICTIONS

- Improvement in NOx & HC emissions
- Mixed results on CO and Soot

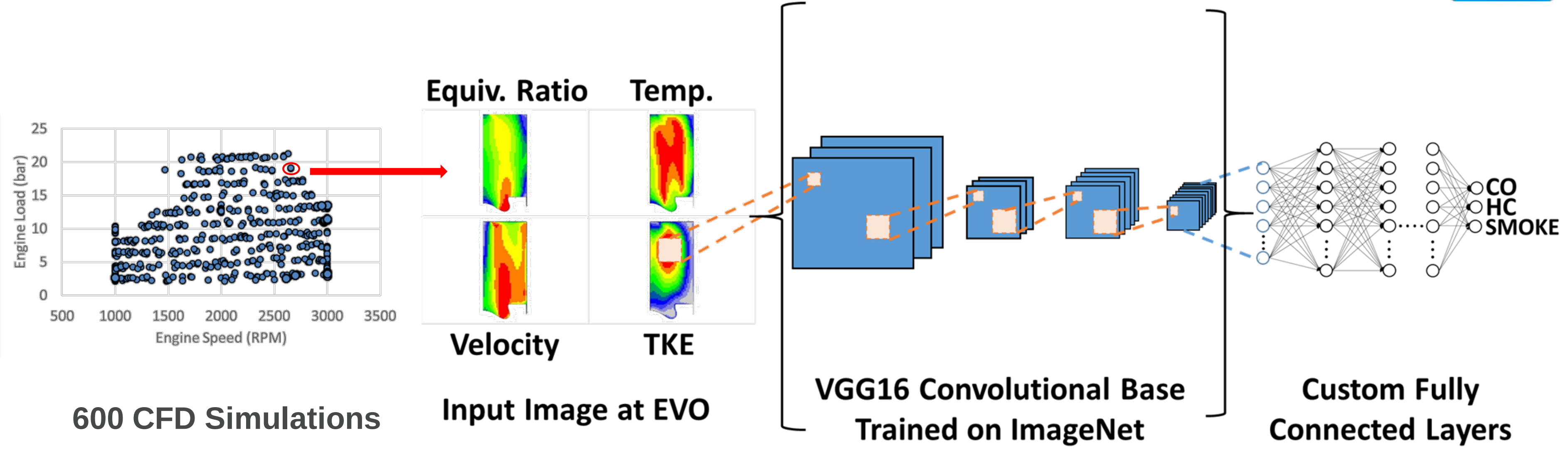


	Baseline	Best Sector	Full-cyl	CHT+RANS
Geometry	Sector	Sector	Cylinder	Engine
Cycle	Closed	Closed	Open	Open
Max # cells	~170k	~1M	~2.5M	~4.5M
# species	47	144	144	144
# reactions	74	900	900	900
NOx	Zel'dovich	GRI 3.0	GRI 3.0	GRI 3.0
Soot	Detailed PSM	Hiroyasu	Hiroyasu	Hiroyasu
Turbulence	RANS	RANS	RANS	RANS
Other changes		Spray and wall-film	Intake swirl vane	CHT
Wall time / cycle	~2 hr	~5 hr	~3.5 days	~2 weeks
Cases	500	602	20	8



DOE Annual Merit Review, 2019

PREDICTION OF ENGINE-OUT EMISSIONS USING DEEP CONVOLUTIONAL NEURAL NETWORKS



Training Data: 400 images

Validation Data: 100 images

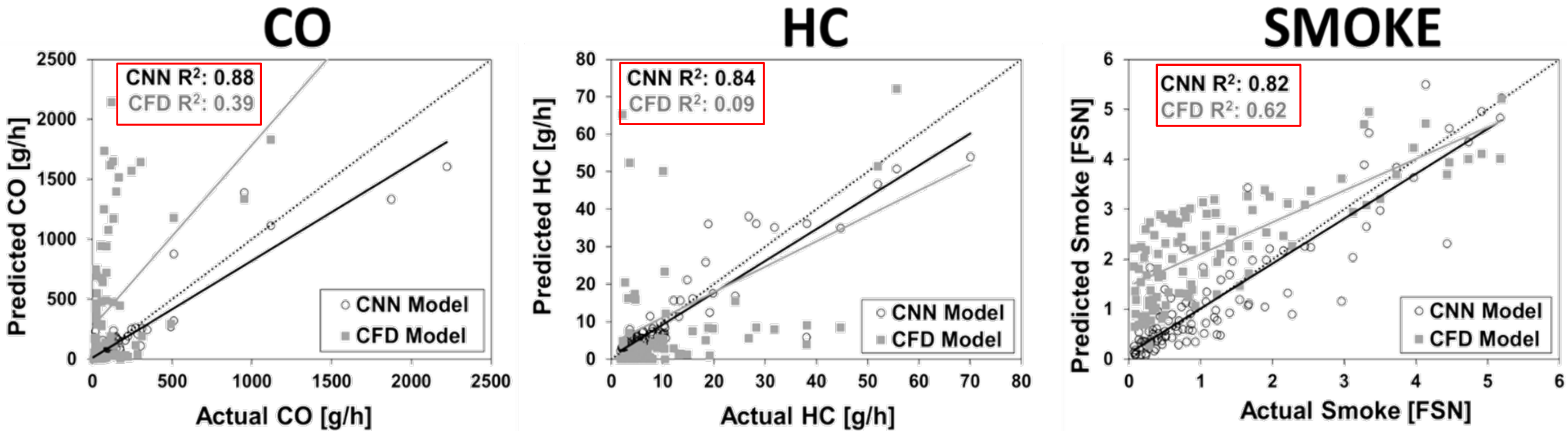
Test or Unseen data: 100 images

Total predicted variables: 3 (CO, HC, Smoke)

SAE 2021-01-0414

CNN VS CFD MODEL PREDICTIONS

CFD model is sector mesh, Hiroyasu Soot model, GRI 3.0 chemistry for NOx

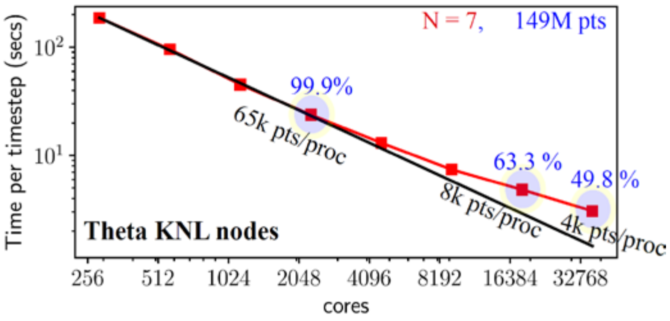


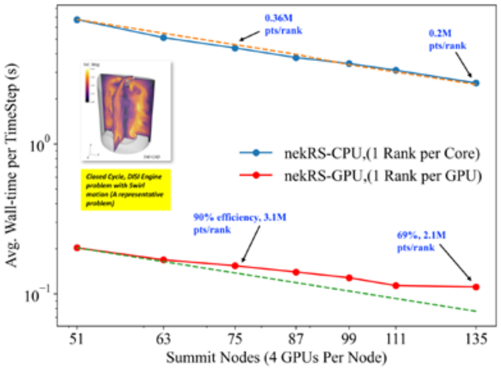
SAE 2021-01-0414

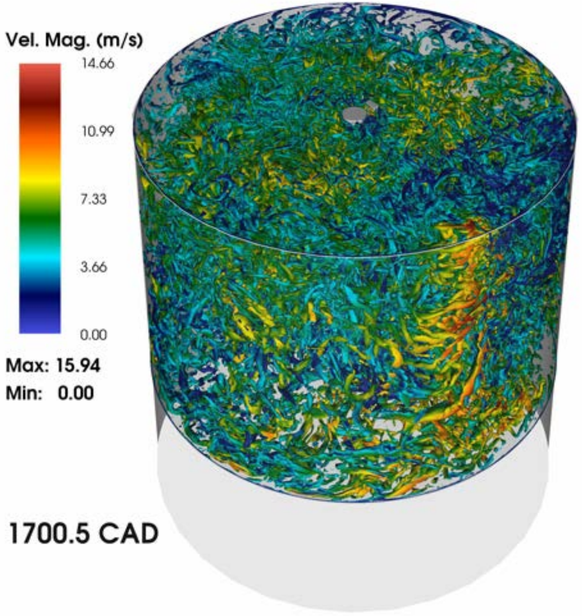
NEW DNS/LES DATA - LEVERAGING EXASCALE COMPUTING

- NEK5000 Spectral element method (SEM) code:
  - High numerical accuracy: N^{th} order tensor-product polynomials (N~ 5-15)
  - Exponential (spectral) convergence with N
  - Handle complex geometries with moving boundaries
  - Efficient scaling on hybrid exascale architectures
- **Objective:** Perform gold-standard DNS/LES simulations for flow and develop/improve submodels for engineering simulations

ENGINE SIMULATIONS ON THETA & SUMMIT SUPERCOMPUTERS



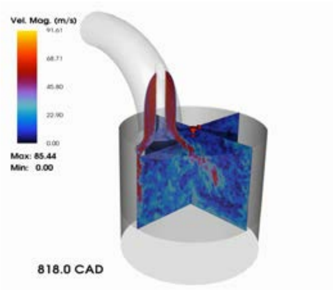




PIs: Muhsin Ameen, Saumil Patel (ANL)

NEW DNS/LES DATA LEADING TO IMPROVED SUB-MODELS

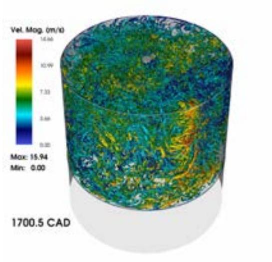
OPEN-CYCLE LES[1]



LES – FUEL INJECTION[2]

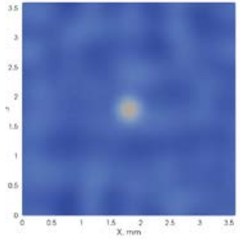
- NEK5000 was used to perform DNS of GM's TCC engine (at University of Michigan) on Theta
  - LES > 95M grid points, scales on >16K procs
  - DNS > 430M grid points, scales on >51K procs

CLOSED-CYCLE DNS



DNS NEAR-SPARK PLUG

DNS – SACI COMBUSTION



- DNS enables development of new heat transfer and combustion models in industry use codes (like CONVERGE) on DOE Exascale machines
- LES framework within the higher order code provides a effective crucible to test efficacy of existing sub-models

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

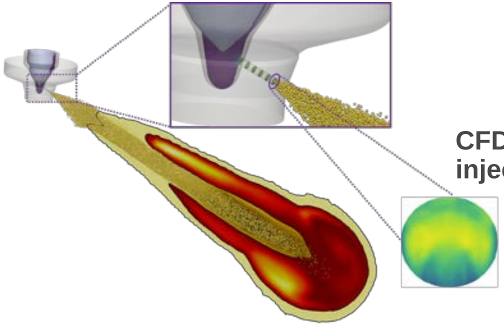
1. S. Wu, M. Ameen, S. Patel, ASME ICEF2021-67671. 2. F. Colmenares, M. Ameen, S. Patel, ASME ICEF 2021-67848

INJECTOR-TO-EMISSION PREDICTION TOOL

Fast and accurate

MACHINE LEARNING ACCELERATES X-RAY TOMOGRAPHY SEGMENTATION

COUPLED INJECTOR-SPRAY SIMULATIONS WITH DETAILED CHEMISTRY[2]



Multiphase Flow Modeling
- Cavitation & erosion
- X-ray scanned geometry
- Transient needle dynamics

+

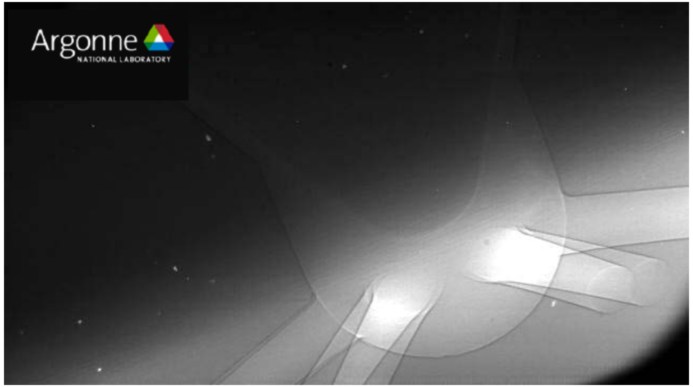
Combustion Modeling
- 2000+ species PAH mechanisms
- Turbulence chemistry interaction
- Detailed surrogates, soot models

>

Coupled Framework
Ability to link injector performance with resultant mixing field, combustion development, and pollutant formation

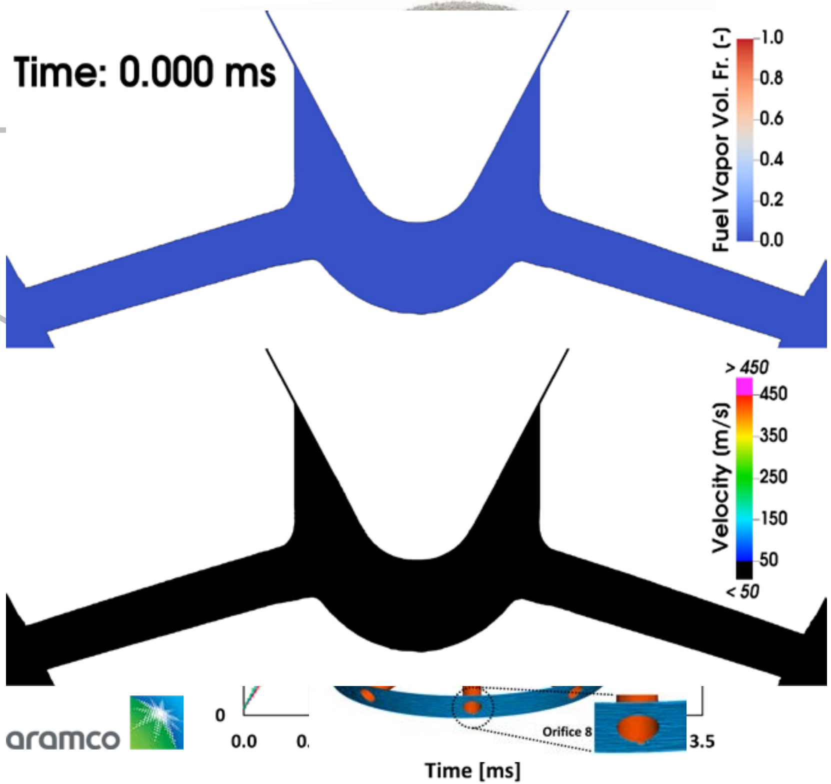
1. Tekawade et al., International Society for Optics and Photonics, 2019. 2. Mondal, Magnotti, Torelli et al., SAE Int. J. Adv. & Curr. Prac. in Mobility, 2021

IN-NOZZLE FLOW SIMULATIONS ACCOUNTING MANUFACTURING TOLERANCES



Video courtesy of Katie Matusik and Chris Powell (Argonne)

- Reconstruction of x-ray scanned geometry
- Extraction of needle motion profiles
- Account for surface finish
- CFD simulations capturing these effects



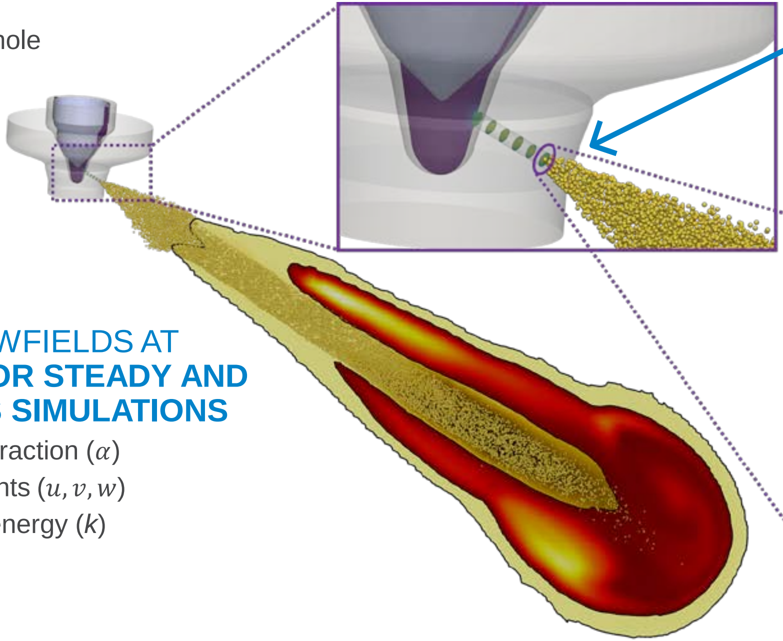
Torelli, Pei, et al. SAE Int. J. Fuels & Lubr. 11(4), 2018

DATA-DRIVEN EMULATOR USED TO PREDICT SPATIOTEMPORAL INJECTION PROFILE

Addresses expense of injector simulations

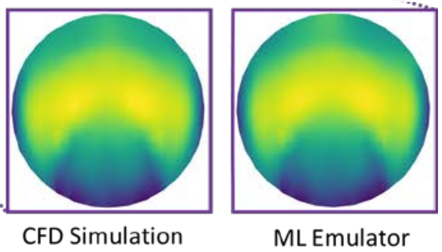
A-M1 INJECTOR

Side-oriented single-hole injector geometry



SIMULATION – DATA – LEARNING (SDL)

- Machine Learning models emulate internal flow fields at orifice exit
- Emulated flowfields coupled with:
  - Lagrangian spray model[1]
  - Eulerian-Lagrangian Spray Atomization (ELSA) model[2]
- Transfer learning underway to extend to other injectors and injection systems



EMULATED FLOWFIELDS AT ORIFICE EXIT **FOR STEADY AND TRANSIENT LES SIMULATIONS**

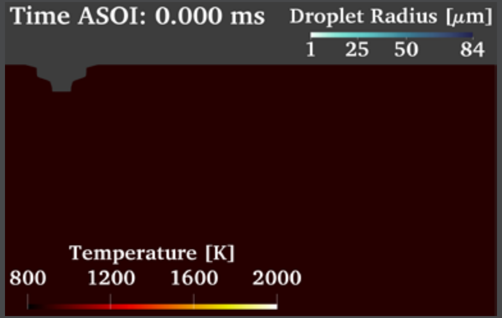
- Gaseous volume fraction (α)
- Velocity components (u, v, w)
- Turbulent kinetic energy (k)
- Liquid mass (m_l)

1. Mondal. Magnotti, Torelli et al., SAE Int. J. Adv. & Curr. Prac. in Mobility, 2021. 2. Magnotti et al., LES4ECE, 2021.

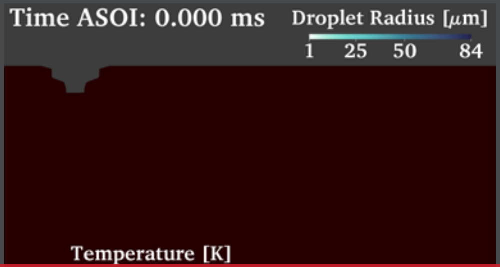
ACCURATE SPRAY COMBUSTION PREDICTIONS AT A FRACTION OF THE COST

Emulator far less expensive than simulating the next point of interest

Injection Map from CFD (“Truth”)

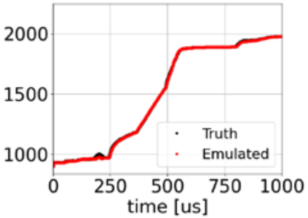


Injection Map from GP-based Emulator

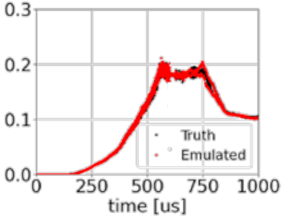


38 MILLION TIMES LESS EXPENSIVE

Max Temperature [K]
Error < 1%

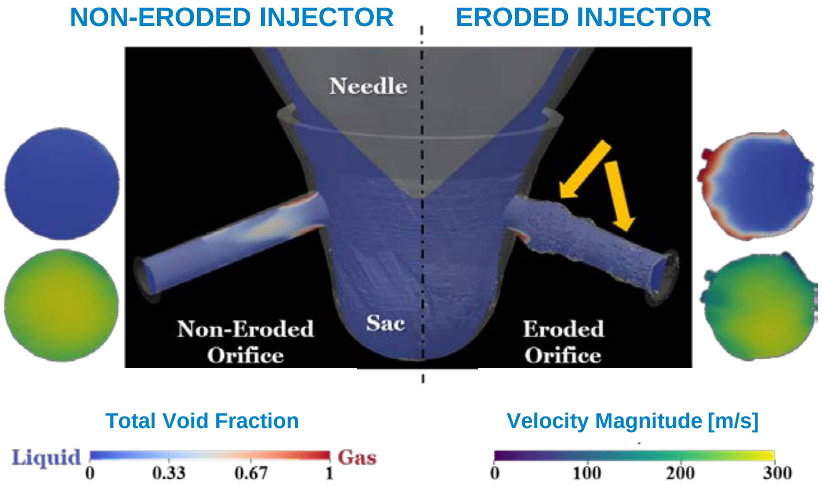


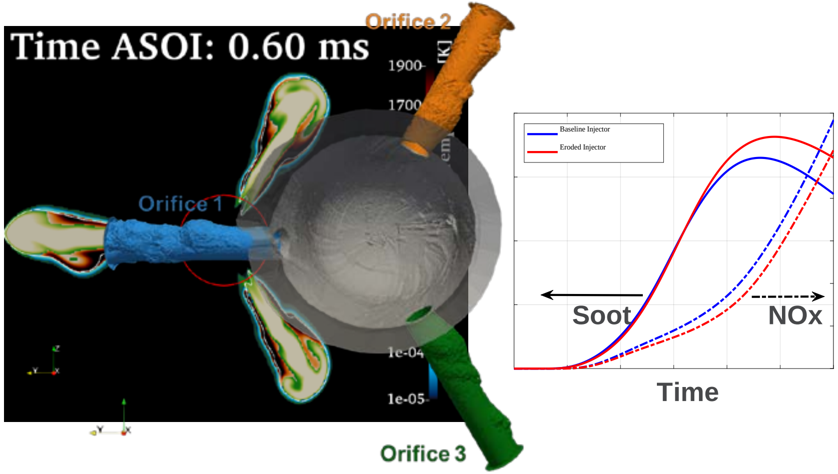
Heat Release Rate [MJ/s]
Error < 1%



1. Mondal, Magnotti, Torelli et al., ASME ICEF 2021-67888, Accepted.

FIRST OF ITS KIND SIMULATION LINKS EROSION FROM AN X-RAY SCANNED INJECTOR WITH SPRAY, COMBUSTION AND EMISSIONS





Internal flow simulations indicate that erosion leads to:

- Increased orifice exit diameter
- Reduction in fuel delivery rates of at least 2 – 3%
- Wider spray spreading angles

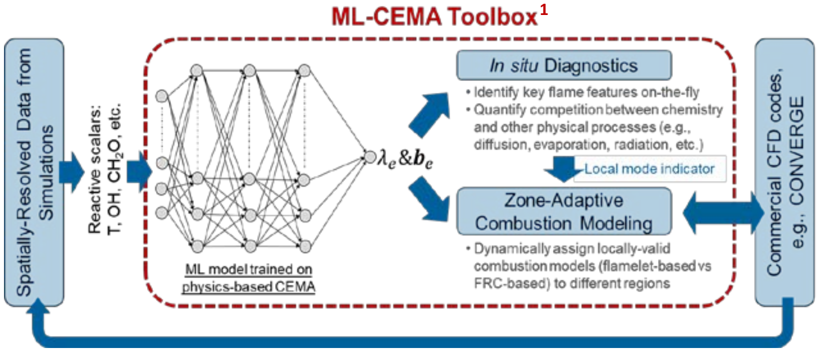
Reacting spray simulations indicate that erosion leads to:

- Similar first and second stage ignition delays
- Shorter flame lift off length
- Higher soot and lower NOx production

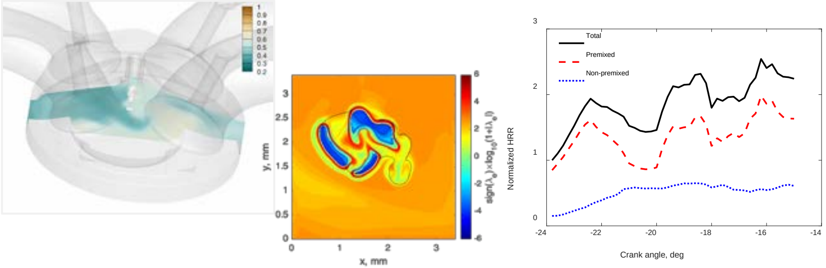
1. Magnotti et al., ASME ICEF 2021-67775, Accepted.

UNIVERSAL COMBUSTION MODEL ENABLED BY ML

- New toolbox **ML-CEMA** (ML-accelerated chemical explosive mode analysis) is developed for **advanced flame diagnostics and modeling.**
- ML-CEMA for any fuel combustion
  - Sheds light on flame stabilization, auto-ignition, flame propagation, extinction, etc.
  - Speed up turbulent combustion modeling (e.g., in LES) **by 4X.**

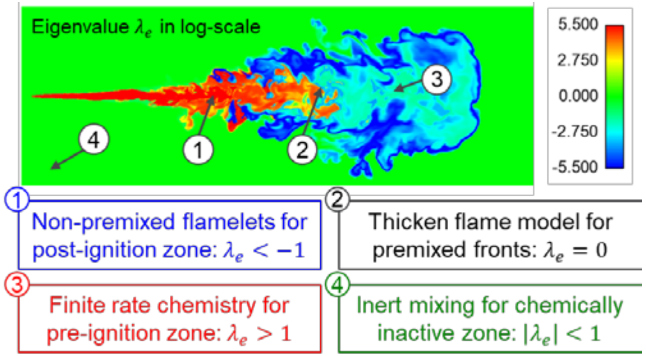


Diagnostics of SACI[2]



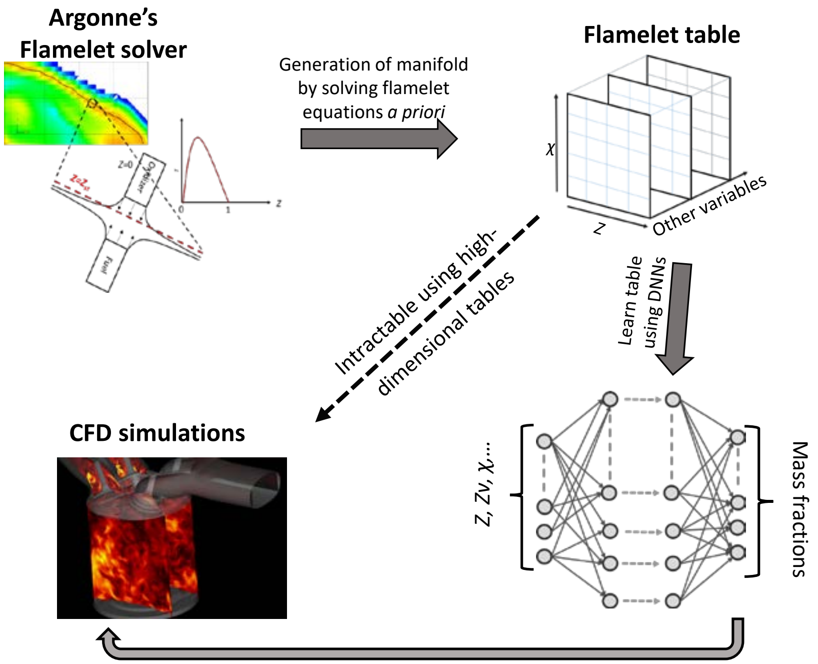
ML-CEMA identifies locations of premixed reaction fronts and distinguishes between premixed and non-premixed flames

Modeling of turbulent partially premixed flames[3]



1. Chao Xu et al, AIAA SciTech 2020. 2. Chao Xu et al, ASME ICEF 2021. 3. Chao Xu et al, CNF 2018

MULTI-COMPONENT DETAILED CHEMISTRY SIMULATIONS ENABLED WITH ANN



1. Kundu et al. Transportation Engineering 2020.
2. Owoyele, Kundu, and Pal, Proceedings of the Combustion Institute, 2020

Argonne's Flamelet Solver together with Unsteady Flamelet Progress Variable (UFPV) model has been extensively validated against engine data with detailed chemistry and soot models[1]

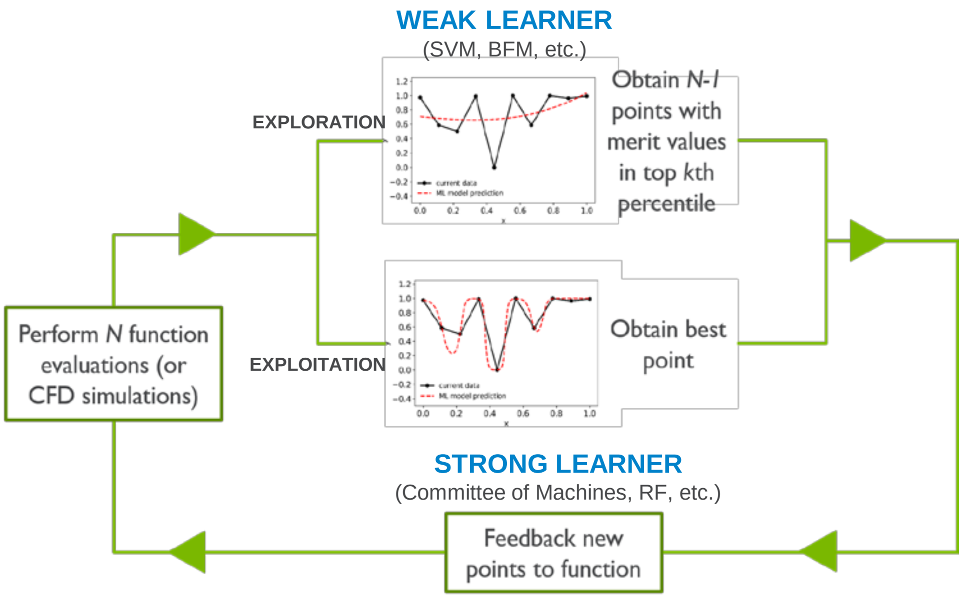
- Accurate predictions in autoignition and unsteady heat release during interaction phase
- Captures both high temperature ignition and low temperature chemistry (LTC)

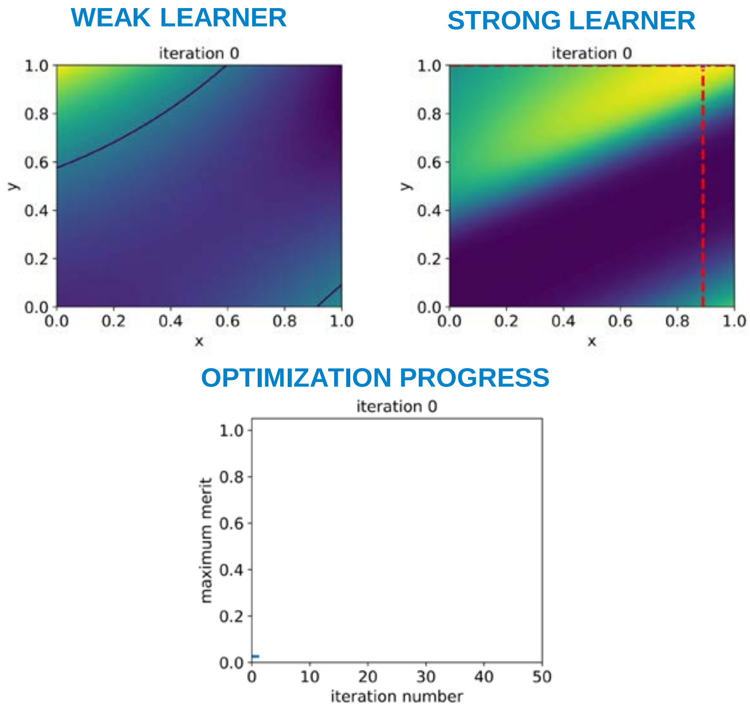
Deep learning techniques further circumvent the issues of high memory footprint and retrieval cost associated with large multi-dimensional flamelet tables

- Mixture of Experts (MoE) approach[2], combining regression and clustering, bifurcates combustion manifolds and learns large flamelet tables
- Allows for incorporation of high-dimensional tables from large chemistry mechanisms

ACCELERATING ENGINE DESIGN OPTIMIZATION WITH ML

ActivO: Basic algorithm

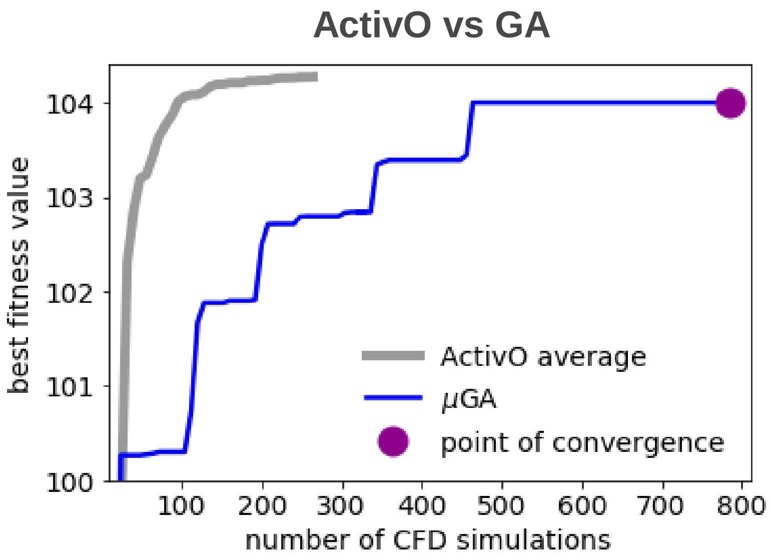




Owoyele & Pal, ASME J. Energy Res. Technol. 2020

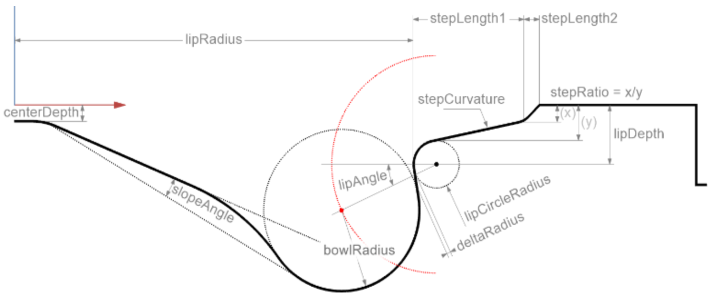
SIMULATION-DRIVEN DESIGN OPTIMIZATION

IC Engine optimization test problem



Owoyele & Pal, Applied Energy, 2021

- Optimization of a heavy-duty engine operating on a gasoline-like fuel to **minimize ISFC** and **adhering to emissions and pressure rise constraints**
- **Nine-dimensional** design space
- Resources reduced from 112000 core hours to 20000 core hours (over 80% decrease)
- Over **5-10x speedup** (from 2 months to less than a week) over traditional algorithms (GA, PSO, etc.)
- **Geometry optimization can also be handled** (*J. Energy Res. Technol. 2020*, SAE 2020-01-1313)



Collaboration with Aramco Research Center-Detroit

GRAND CHALLENGE PROBLEMS IN 5-15 YEARS THAT HPC & AI/ML CAN HELP SOLVE

- Multi-cycle, multi-cylinder simulations including conjugate heat transfer and TCI modeling for future low-Carbon/no-Carbon fuels (24-hour turn-around time)
- Coupled multi-scale modeling of two-phase fuel injection with engine combustion and after-treatment systems
  - Cold start emission predictions
- Predicting cyclic variability and understanding root causes
  - Engine knock/misfire, i.e., rare event detection
- DNS/high-fidelity LES for HD, Rail, Marine – well beyond exascale computing

CATEGORY	DOMAIN VOLUME (L)		RANS	LES	DNS
Light Duty	0.6315	Mesh size (mm)	0.5	0.015	0.009
		Cell count (Millions)	2	100	416
		Core hours (Millions)	0.035	1.9	3.7
Heavy Duty	2.5	Mesh size (mm)	0.35	0.02	0.01
		Cell count (Millions)	3.1	296.9	1482
		Core hours (Millions)	0.12	7.5	14.6
Rail	16.6	Mesh size (mm)	0.5	0.03	0.015
		Cell count (Millions)	52.6	2629	10935
		Core hours (Millions)	0.92003	49.9	97.3

Estimated computing cost per production simulation

4-cycle Progress Rail H Engine at Argonne (16.6 L)

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THANK YOU

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