REIMAGINING IC ENGINE DEVELOPMENT LEVERAGING NEXT-GENERATION HPC & AI

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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

Goal: First time capable designs to reduce iterations in the physical world

HPC Growth & Reduction in Hardware

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

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<td>ORNL</td>
<td>AURORA</td>
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EXASCALE SYSTEMS
FOUR PRIMARY ALLOCATION PROGRAMS

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

- **10%** Director’s Discretionary
- **Up to 20%** ECP Exascale Computing Project
- **20%** ALCC ASCR Leadership Computing Challenge
- **50%** INCITE Leadership Computing
TOWARDS PREDICTIVE ENGINE SIMULATIONS

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

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

Design new experiments / condition

PELE
DNS of engine condition

Initial & Boundary conditions

NEK5000
DNS & LES of PACE engines

SOFTWARE TECHNOLOGIES
Math libraries, Co-design, ...

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)
High-fidelity wall-resolved LES at limited conditions

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

High-throughput design space exploration – RANS

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

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

DNS for generating gold-standard datasets at select conditions

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

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

HPC simulations provide a benchmark for accuracy of engineering simulations

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)
EXAMPLE OF CAPABILITY COMPUTING

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

### Geometry Sector

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Sector</th>
<th>Best Sector</th>
<th>Full-cyl</th>
<th>CHT+RANS</th>
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<tr>
<td>Cycle</td>
<td>Closed</td>
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<td>~170k</td>
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<td>Detailed PSM</td>
<td>Hiroyasu</td>
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<td>RANS</td>
<td>RANS</td>
<td>RANS</td>
<td>RANS</td>
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<td>Other changes</td>
<td>Spray and wall-film</td>
<td>Intake swirl vane</td>
<td>CHT</td>
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<tr>
<td>Wall time / cycle</td>
<td>~2 hr</td>
<td>~5 hr</td>
<td>~3.5 days</td>
<td>~2 weeks</td>
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<tr>
<td>Cases</td>
<td>500</td>
<td>602</td>
<td>20</td>
<td>8</td>
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### Cases

- Cases 500
- Cases 602
- Cases 20
- Cases 8

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### Figures

- Engine Load vs. RPM
- Emission predictions for NOx, HC, CO, and Soot.
PREDICTION OF ENGINE-OUT EMISSIONS USING DEEP CONVOLUTIONAL NEURAL NETWORKS

600 CFD Simulations

Equiv. Ratio  Temp.
Velocity  TKE

Input Image at EVO

VGG16 Convolutional Base Trained on ImageNet

Custom Fully Connected Layers

Training Data: 400 images
Validation Data: 100 images
Test or Unseen data: 100 images
Total predicted variables: 3 (CO, HC, Smoke)
CNN VS CFD MODEL PREDICTIONS

CFD model is sector mesh, Hiroyasu Soot model, GRI 3.0 chemistry for NOx
NEW DNS/LES DATA - LEVERAGING EXASCALE COMPUTING

- NEK5000 Spectral element method (SEM) code:
  - High numerical accuracy: $N^{th}$ order tensor-product polynomials ($N \sim 5-15$)
  - 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

Plots: Muhsin Ameen, Saumil Patel (ANL)
NEW DNS/LES DATA LEADING TO IMPROVED SUB-MODELS

- 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

- 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 an effective crucible to test efficacy of existing sub-models

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

Computed Tomography (CT) Slice

COUPLED INJECTOR-SPRAY SIMULATIONS WITH DETAILED CHEMISTRY

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

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

Video courtesy of Katie Matusik and Chris Powell (Argonne)

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
  - Eulerian-Lagrangian Spray Atomization (ELSA) model
- 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 ($\alpha$)
- Velocity components ($u, v, w$)
- Turbulent kinetic energy ($k$)
- Liquid mass ($m_l$)

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

Max Temperature [K]
- Error < 1%

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

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

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

3. Chao Xu et al, CNF 2018
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

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\(^1\) Kundu et al. Transportation Engineering 2020.
\(^2\) Owoyele, Kundu, and Pal, Proceedings of the Combustion Institute, 2020
ACCELERATING ENGINE DESIGN OPTIMIZATION WITH ML

ActivO: Basic algorithm

WEAK LEARNER
(SVM, BFM, etc.)

Obtain N-1 points with merit values in top kth percentile

STRONG LEARNER
(Committee of Machines, RF, etc.)

Feedback new points to function

Perform N function evaluations (or CFD simulations)

EXPLORATION

EXPLORATION

EXPLOITATION

Obtain best point

OPTIMIZATION PROGRESS

IC Engine optimization test problem

- 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)
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

<table>
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<tr>
<th>CATEGORY</th>
<th>DOMAIN VOLUME (L)</th>
<th>Mesh size (mm)</th>
<th>RANS</th>
<th>LES</th>
<th>DNS</th>
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Estimated computing cost per production simulation

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

SPONSORS
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