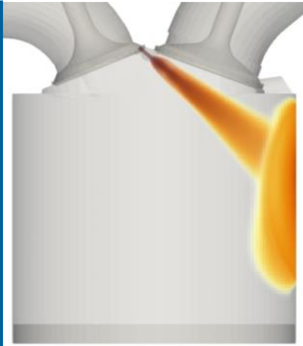
COMPUTATIONAL MODELING OF LOW-C FUELS COMBUSTION FOR PROPULSION AND POWER



Riccardo Scarcelli, Group Leader

Multi-Physics Engine Computations, Center for Advanced Propulsion and Power

Transportation and Power Systems Division, Argonne National Laboratory

KAUST Research Conference Hydrogen-Based Mobility and Power

KAUST, October 23-26, 2022

MULTI-PHYSICS COMPUTATIONS SECTION AT ARGONNE

MULTI-PHYSICS COMPUTATIONS SECTION

Director,
Center for Advanced Propulsion and Power (CAPP)

Group Leader,
Multi-Physics Engine Computations

Research Scientists

Postdocs

GTs, RDEs, Scramjets | **Piston Engines**

- **Core Capabilities & Model Developments:**
  - Exascale Computing with high-order Nek5000 code, Multi-phase and Reacting flow modeling, AI/ML for fast/efficient design.
- **HPC for multi-scale, multi-physics applications serving DOE offices, DOD agencies, and industry:**
  - Piston Engines, Gas Turbines (GTs), Rotating Detonation Engines (RDEs), Scramjets, etc.
  - Electric motor cooling, External aerodynamics, Heat exchangers, Energy storage in phase change materials, Manufacturing processes, Electrospinning, Carbon capture, Heat pumps, After-treatment devices, Burners, and several other applications.

COMPUTING CONTINUUM @ ARGONNE

Next-gen supercomputers

2017-present

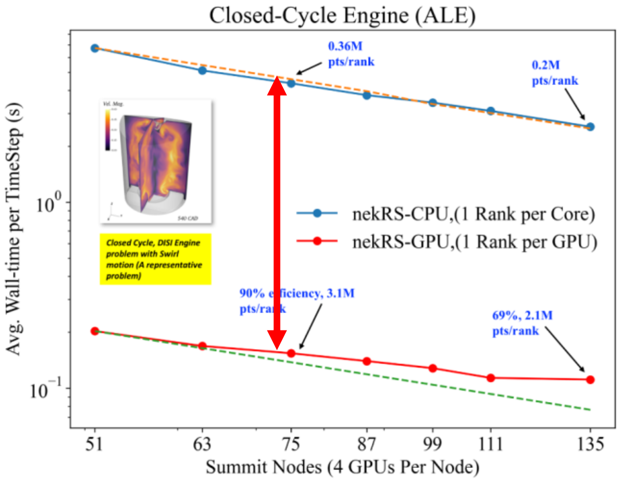
Theta/Theta-GPU

2021

Polaris (GPU only)

2022

Aurora: Exascale Machine

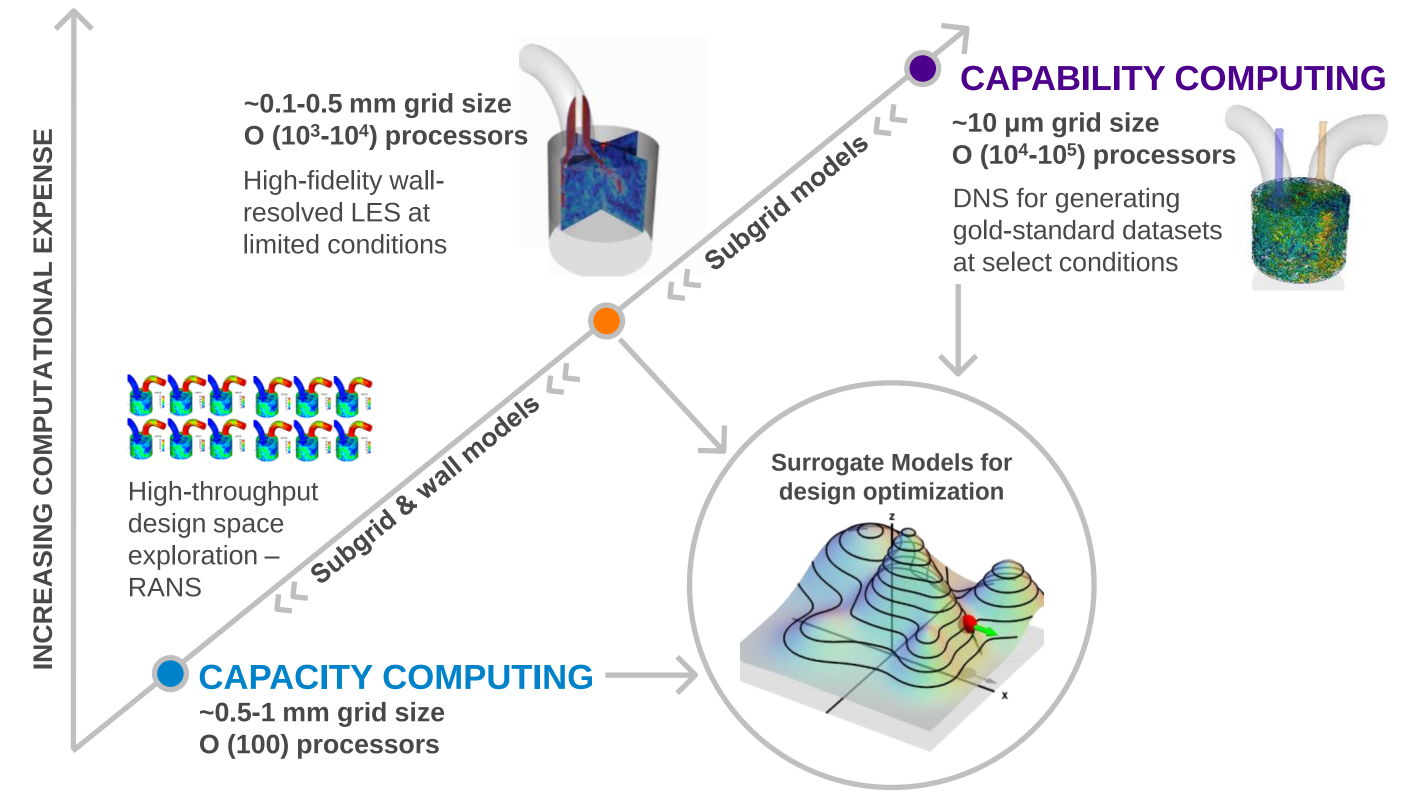


GPUs provide 10-15x speed-up over CPU

Ameen et al., DOE Advanced Engine Combustion Review Meeting, Aug 10-13, 2021

- **Connected file systems** for efficient work and data sharing across multiple resources.
- **Multiple hybrid HPCs**: Theta-GPU (3.9 petaflops), Polaris (44 petaflops), Aurora (1 exaflops).
- Development of **GPU-ready nekRS for DNS @ Exascale.**
- One of lead labs of **AI for Science** Initiative (https://www.anl.gov/ai-for-science-report)
- Testbed for **Emerging AI hardware** (https://ai.alcf.anl.gov/#systems)

VISION: MULTI-FIDELITY MODELING FRAMEWORK



LEVERAGE A MULTI-FIDELITY SIMULATION FRAMEWORK TO:

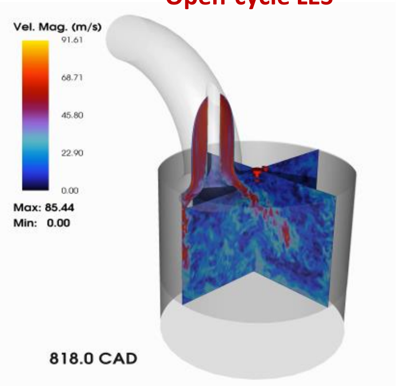
- Improve understanding of flow and combustion processes
- Develop physics-based and data-driven subgrid models
- Perform simulation-based design optimization
- Develop surrogate models for fast design optimization

GOLD-STANDARD DNS/LES

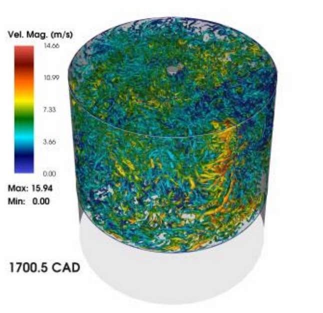
Nek5000/nekRS: Exascale CFD code (ECP-funded)

- High-order in space (spectral element method, 5th - 15th order) and in time (up to 3rd order) with new capability to capture compressibility effects.
- Body-fitting capabilities for complex geometries.
- Arbitrary Lagrangian Eulerian capabilities to handle moving geometries.
- Overset mesh capability to handle multiple overlapping meshes.
- Demonstrated scalability on more than **500,000** processors.
- nekRS - the GPU variant of Nek5000:
  - One of few GPU-ready exascale codes under active development leveraging ~$15M ASCR investment.
  - 10-15 times speedup compared to Nek5000.
  - Scales on ~30,000 GPUs.
- Ideal for **gold-standard DNS/LES** for complex flow problems and develop/improve **physics and ML based models.**

Open-cycle LES

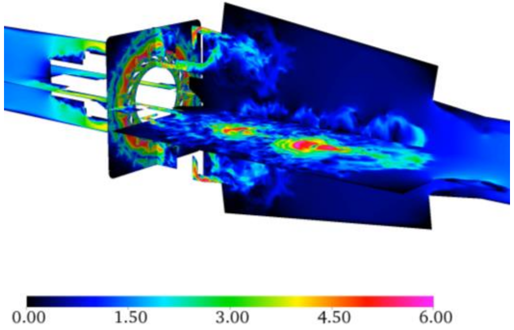


Closed-cycle DNS



LES > 95M grid points

DNS > 430M grid points

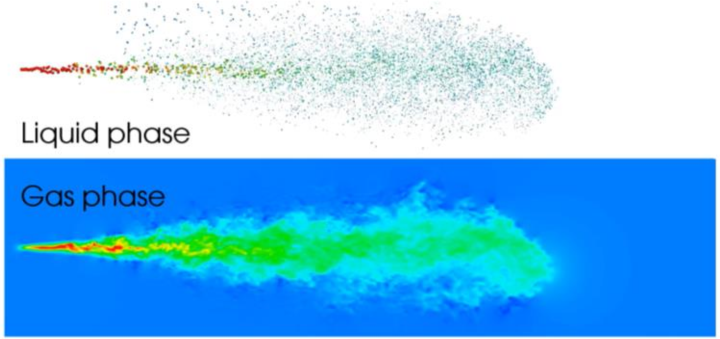


DNS > 350M grid points

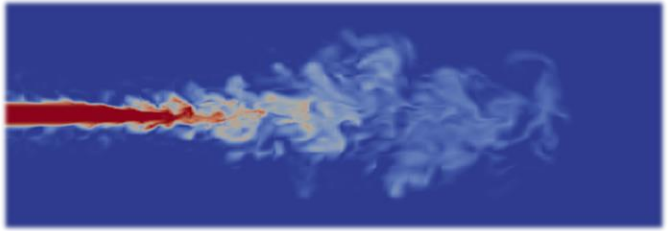
CFD MODEL DEVELOPMENT USING DNS/LES

Predictive sub-models to improve simulation accuracy

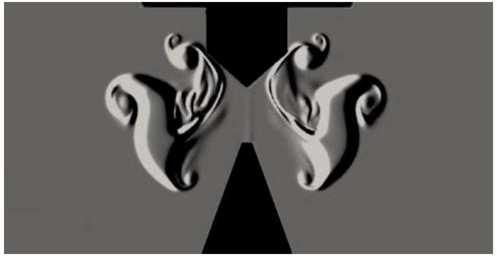
Multi-phase flow
- Droplet velocity, size distribution, spray con angle.
- Cavitation, erosion / spray-wall interaction.

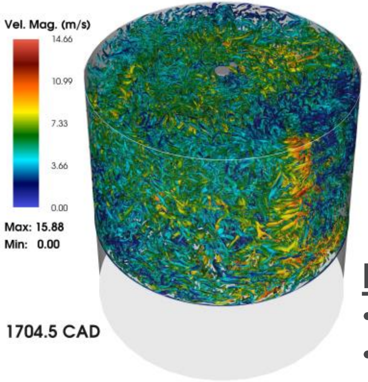


Gas injection & mixing
- Gas-jet structure, mixing w/ surrounding gas.

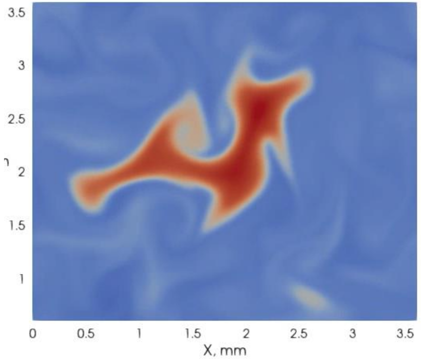


Ignition
- Arc elongation, restrike.
- Flame kernel evolution.





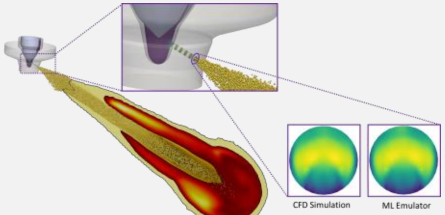
Combustion
- Turbulent combustion with deflagration, auto-ignition.
- Flame instabilities, lean blow-out, lift-off length.
- Abnormal combustion.

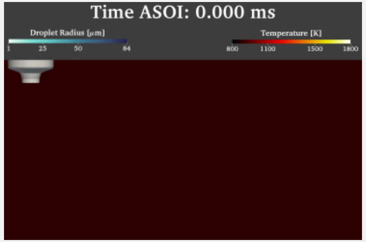


Heat transfer
- Surface roughness.
- Conjugate heat transfer.

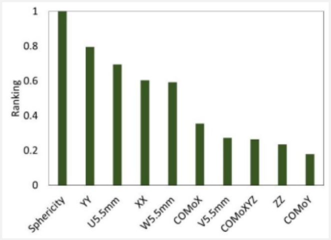
OVERVIEW OF MACHINE LEARNING CAPABILITIES

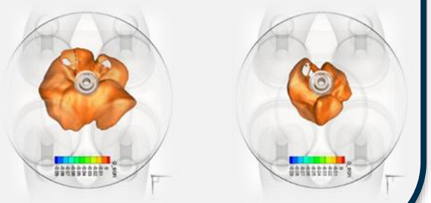
ML-driven CFD surrogate development



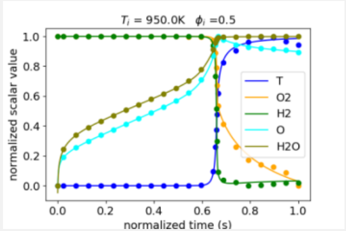


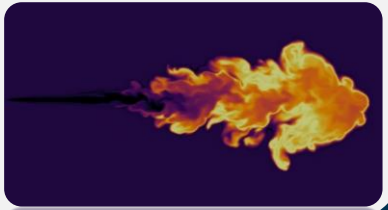
AI-driven understanding of rare-events in engines



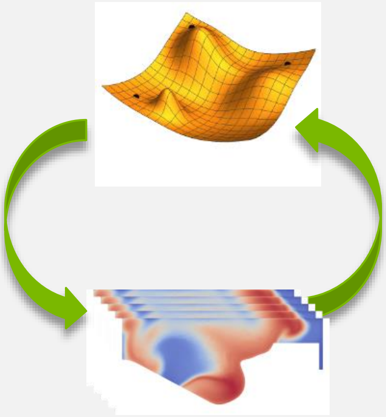


Deep learning augmented chemical kinetics solvers





Ensemble ML + Active Learning for efficient engine design optimization



Unsupervised: dimensionality reduction and anomaly detection

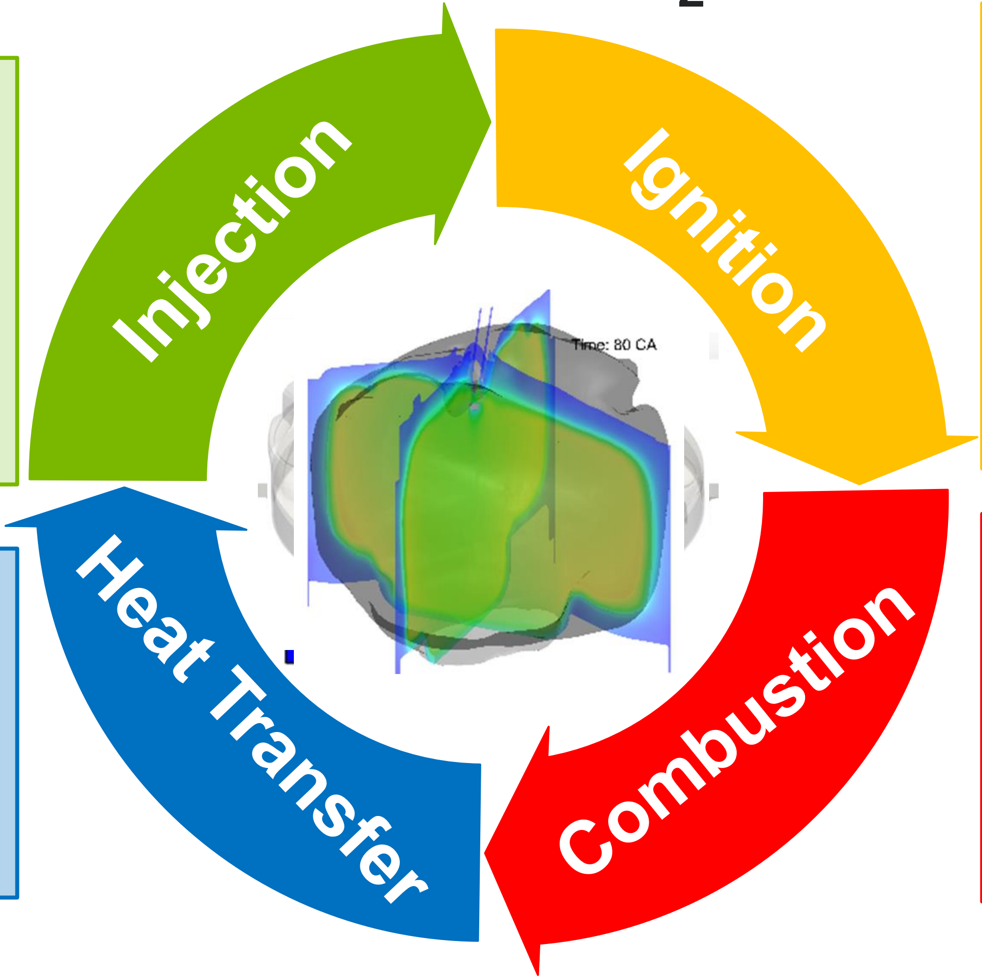
Supervised: classification

Supervised learning: regression

MODELING H_2 RECIP. ICEs FOR PROPULSION AND POWER

CFD MODELING NEEDS FOR H_2 RECIP. ICEs

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



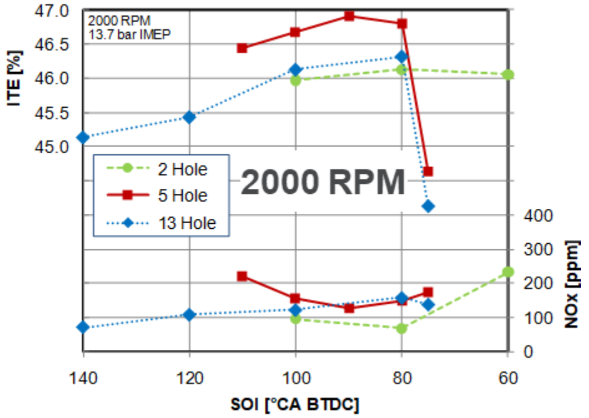
Ignition
- Conventional SI (discharge model, flame kernel growth).
- Advanced ignition (discharge model, flame kernel growth, turbulence, kinetics).
- Diesel pilot (spray models, mixing model, kinetics).

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

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

DIRECT INJECTION OF H_2 FOR RECIP. ICEs

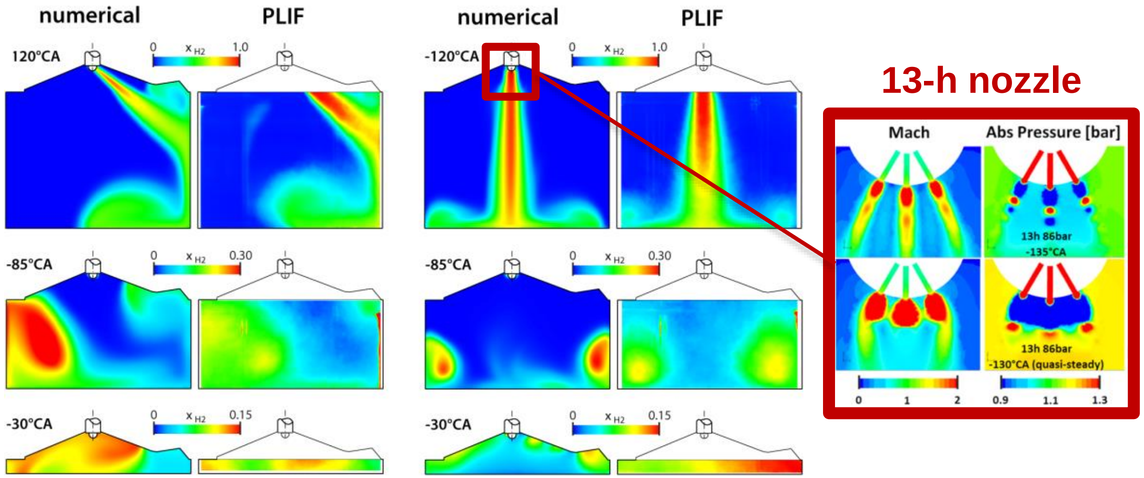
Impact of DI strategies on efficiency/emissions



- Argonne led high-efficiency H_2 ICE light-duty research for DOE between 2005 and 2012, in collaboration with Sandia, Ford, Westport.
- Several injector nozzle configurations tested by CFD.
- Met all the goals set by DOE:
  - 45.5% BTE_{PEAK}, 33.3% BTE at WWMP
  - 14.3 bar BMEP, emissions within SULEV

CFD model validation

- Accurate prediction of the gas-jet penetration and evolution during compression stroke.
- Under-prediction of mixing between injected fuel and ambient gas.
- Complex geometries worsened agreement (jet-to-jet interaction).

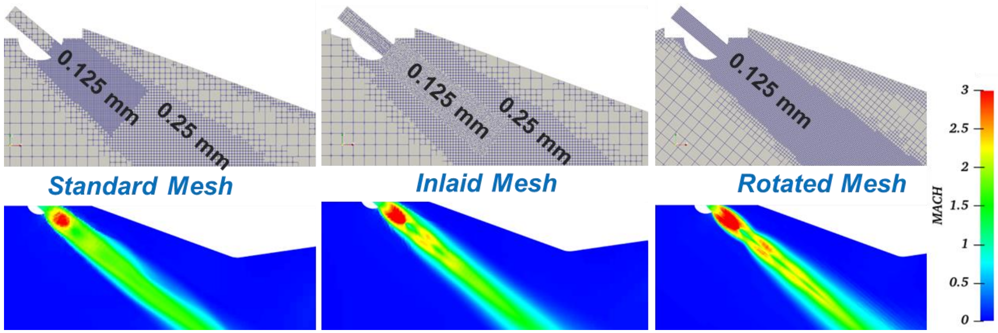


PLIF data from SNL: https://ecn.sandia.gov/engines/hydrogen-engine/

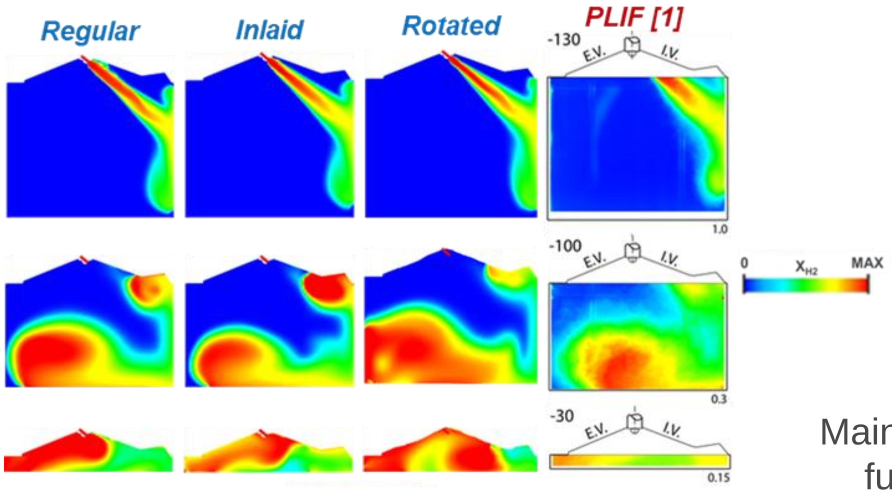
RECENT PROGRESS ON DI H_2 ICE MODELING

Impact of meshing strategies

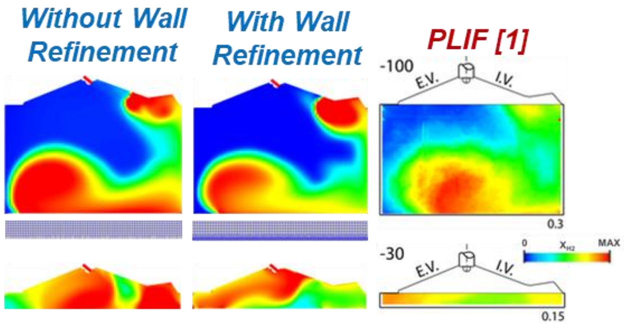
- Best mesh strategies (inlaid mesh) delivers improved agreement with optical data in terms of initial jet behavior (penetration and impingement on walls).
- Rotated mesh loses its advantage after the gaseous jet impinges on the wall (mesh not aligned to the wall).
- Mesh alignment and refinement along the walls proved to be effective in improving CFD results.



Standard Mesh **(Cost: 100%)** ***Inlaid Mesh*** **(Cost: 92%)** ***Rotated Mesh*** **(Cost: 86%)**



[1] https://ecn.sandia.gov/engines/hydrogen-engine/



Main Conclusion: Despite significant improvements, <u>fuel/air mixing continues to be under-predicted</u>

U.S. DEPARTMENT OF ENERGY Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

Work in collaboration with Aramco Research Center – Detroit and funded by Aramco Americas

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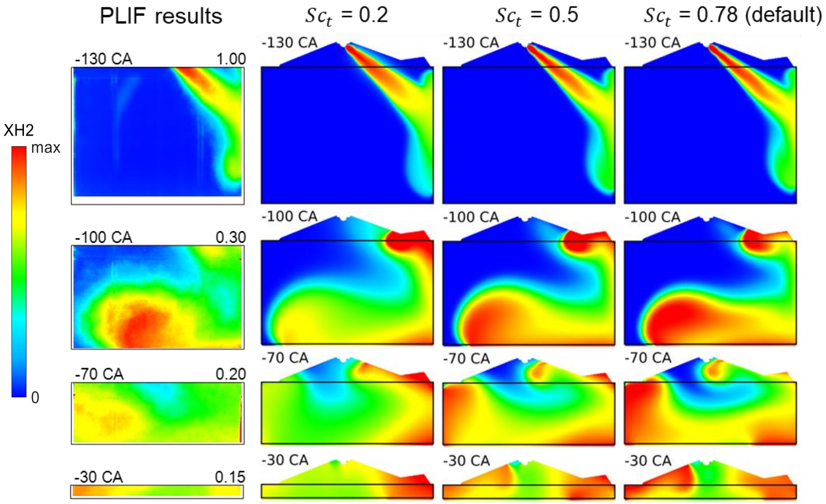
RECENT PROGRESS ON DI H_2 ICE MODELING

Impact of turbulence modeling



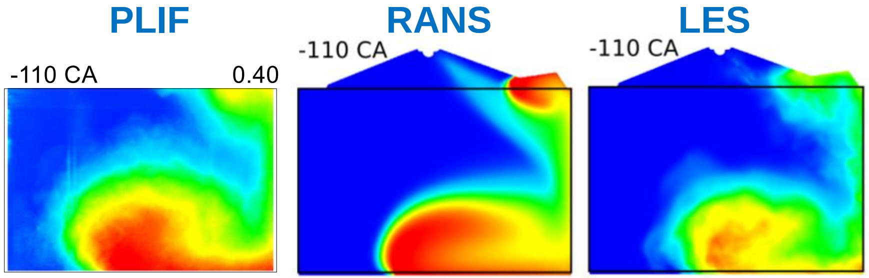
Impact of Turbulent Schmidt number:

$$Sc_t = \nu_t / D_t$$

- Closer agreement of H_2 recirculation cloud at early stage is observed with $Sc_t = 0.5$.
- Reducing Sc_t increases the fuel dispersion due to enhanced diffusion. $Sc_t = 0.5$ is suggested.
- Further investigation (e.g., higher fidelity simulation) is conducted to improve prediction of fuel dispersion.

Future directions:

- Evaluate LES + finer meshes to improve mixing.
- Preliminary results with LES are very encouraging.



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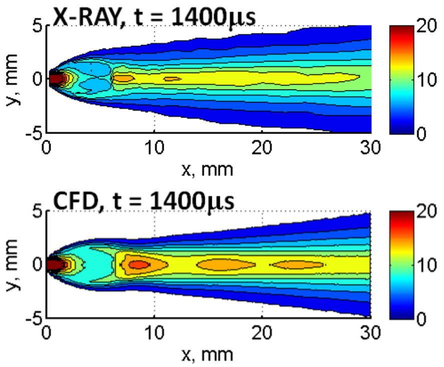
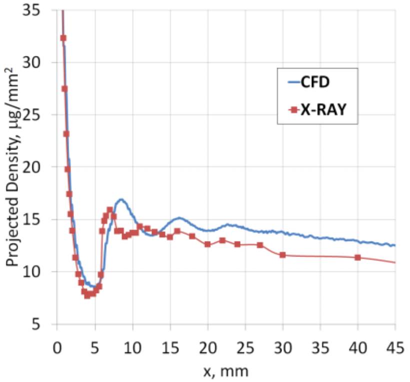
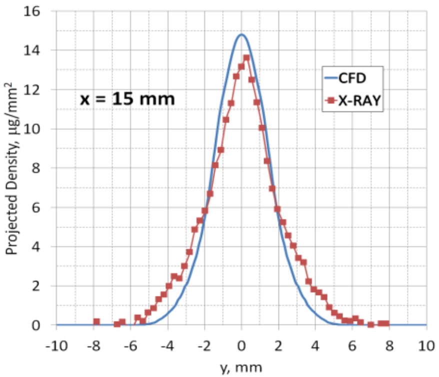
UNDER-EXPANDED GAS-JET MODELING

Validation of CFD results against high-fidelity X-ray diagnostics





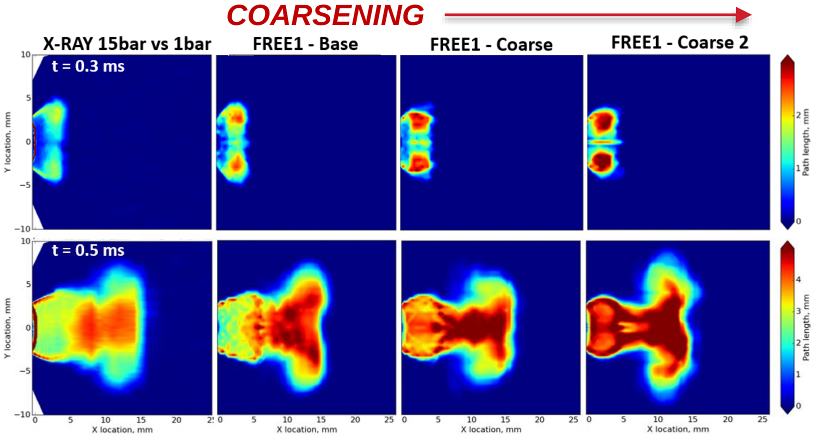


High-pressure DI

- Inward opening injector.
- Argon gas injected at 100 bar.
- Ma disk location well captured.
- Shock structure fairly captured.
- Gas-jet mixing poorly captured (especially in the far field).

Low-pressure DI

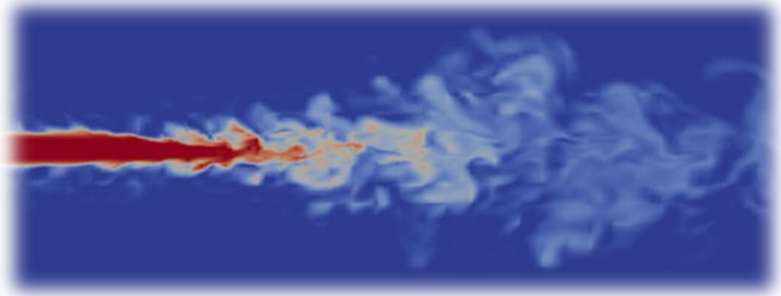
- Outward opening injector.
- Argon gas injected at 10-15 bar.
- Good validation against X-ray for ≈15-30μm meshes.
- Coarsening the mesh makes the agreement worse.
- Typical CFD engine simulations use much less fine meshes (≈ 100-200μm).

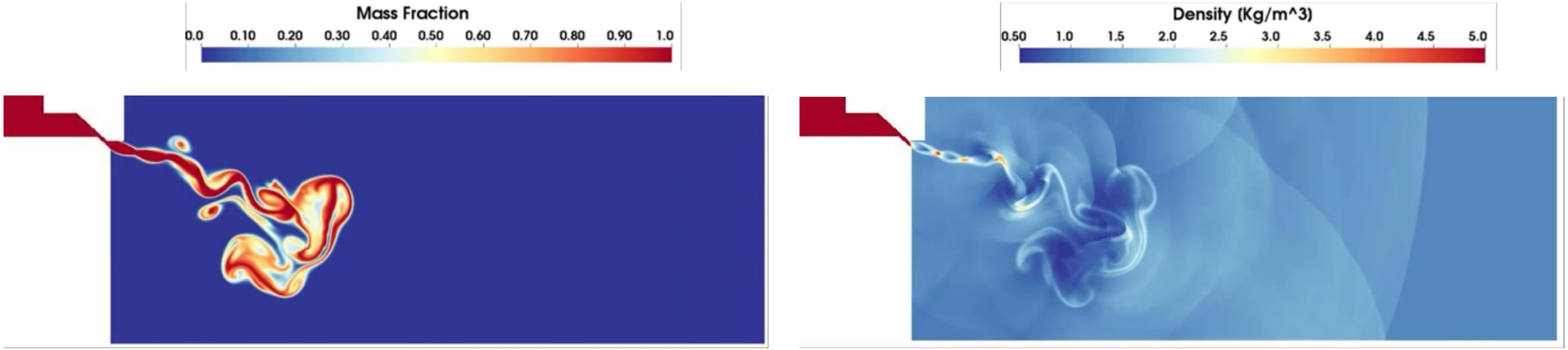


X-ray data: Courtesy of C. Powell (ANL)

H_2 DI/MIXING MODEL DEVELOPMENT

- Leverage recent developments in fully-compressible Nek5000 version to capture shock structure of under-expanded jets.
- DNS can support the development of LES/RANS sub-models to improve CFD predictions of fuel/air mixing processes.
- Initial 2-D DNS calculations carried out to evaluate impact of flow conditions (pressure ratio, velocity, etc.) on the shock structure and mixing between gaseous jet and ambient gas.





Instantaneous mass fraction and density from 2-D Nek DNS of the injector opening transient (pressure ratio = 15:1)

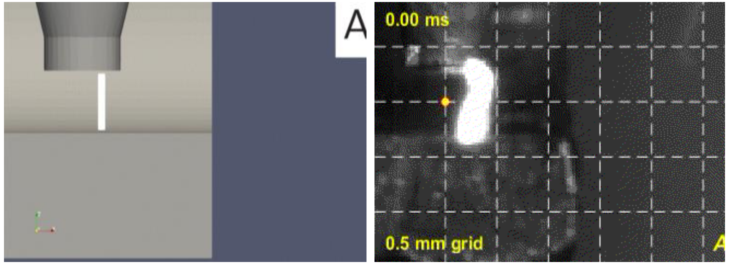
ADVANCED IGNITION MODELING

High-fidelity CFD models for spark-ignition processes

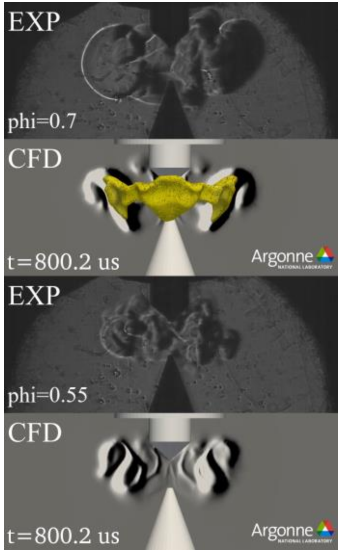
Spark-ignition event in a cross flow

Schlieren data from our partners at MTU, SNL, Stellantis

Ignition Source Evolution



Flame kernel growth



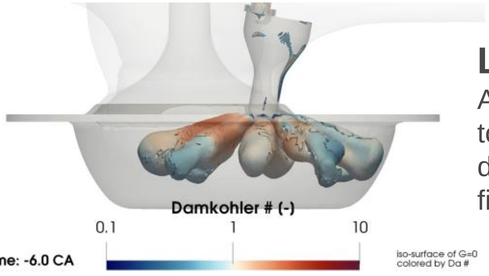
Lagrangian Eulerian Spark-Ignition (LESI) Model

- Fully developed circuit modeling capabilities.
- Coupled with LES/RANS combustion models (G-Eq, TFM, WSR).
- Ready for simulating complex devices (e.g., IC engines).

Engineering CFD models for alternative ignition

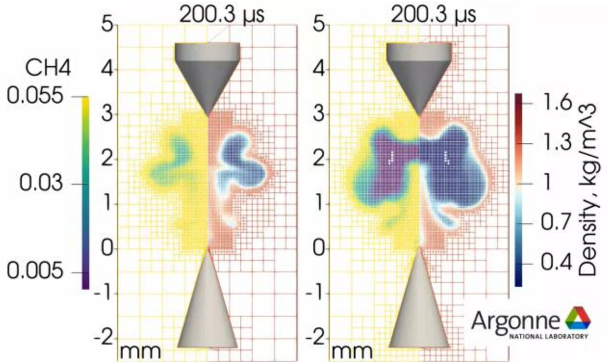
Pre-Chamber SI

Leverage existing SI combustion models and defines best-practices to simulate PC SI engines.



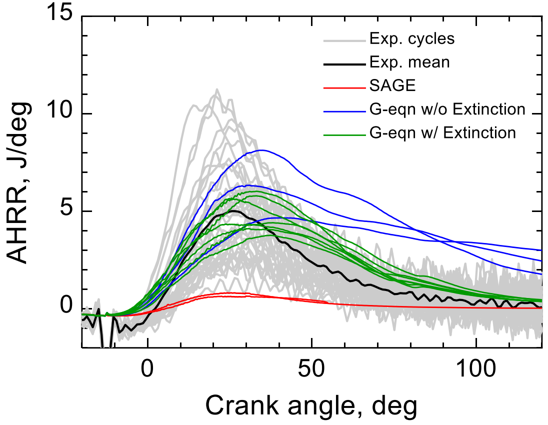
LTP Ignition

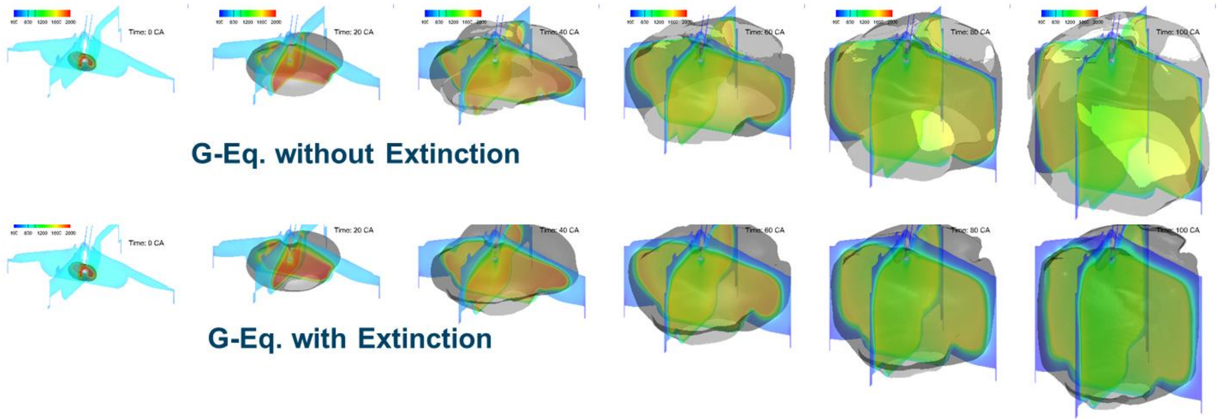
Advanced deposition model to mimic multi-pulse LTP discharge. Leverage high-fidelity plasma simulations.



FLAME WALL QUENCHING MODELING

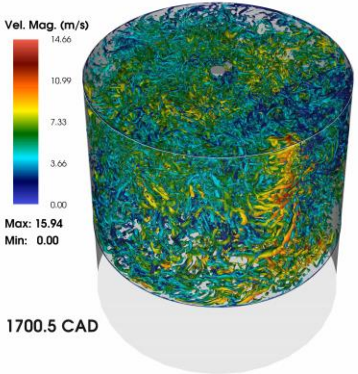
- G-Equation is a commonly-used model for under-resolved turbulent premixed flames.
- Flame-wall interaction is important as flame propagates toward cylinder walls.
- The quenching distance δ_Q is proportional to laminar flame thickness:
  - $\delta_Q = P_e \delta_f$
- The G-Eq. model available in CONVERGE is not able to predict the flame quenching when flame approaches the wall.
- A flame quenching model based on:
  - Large heat loss when flame is too close to the wall ($y_w < P_e \delta_f$)
  - Extremely large local Karlovitz number ($\mathrm{Ka}_\delta > \mathrm{Ka}_\delta^{crit}$)
- The new model was implemented in CONVERGE using UDFs.

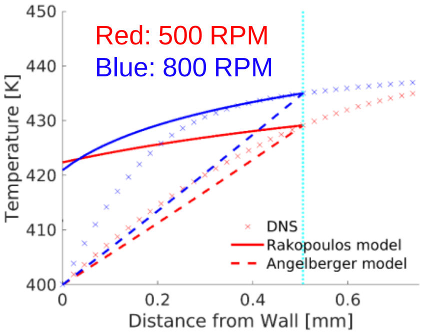


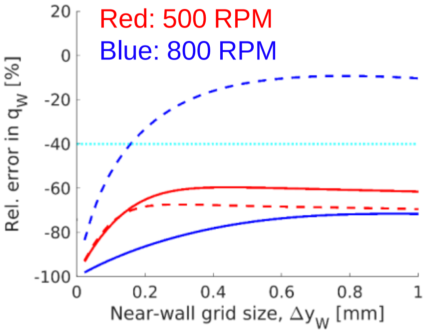


HEAT TRANSFER MODELING

- Performed the first ever DNS of compression/expansion of TCC-III motored operation at 500-800 RPM.
- Validated the flowfield and heat transfer using experimental measurements to increase confidence in the accuracy of the DNS.





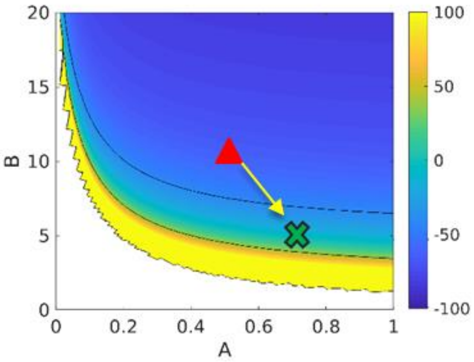


- A-priori evaluation of the accuracy of existing wall models.
- Model error for Rakopoulos model as a function of near-wall grid size.

- **Objective**: Tune model parameters in the Rakopoulos model formulation to improve wall heat flux prediction by using DNS:

$$T^+ = \frac{1}{A}\log\left(y^+ + \frac{1}{APr}\right) - \frac{1}{A}\log\left(40 + \frac{1}{APr}\right) + B$$

- Performed optimization of the Rakopoulos heat transfer model using DNS data.
- Changing (A,B) from (**0.4747,10.2394**) to (**0.7,5.0**) reduced model error to < 30% for near-wall grid sizes < 1 mm across different RPMs and CADs.

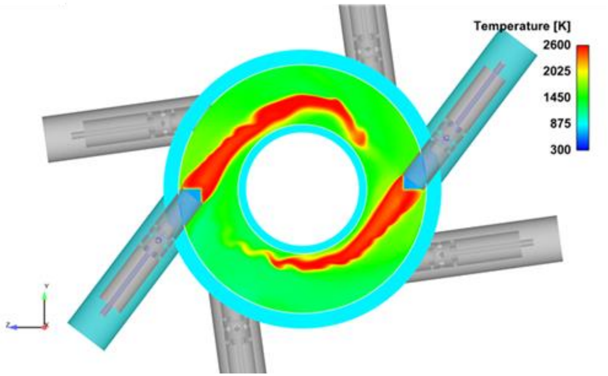


H_2 COMBUSTION FOR NON-ICE APPLICATIONS

H_2-NG COMBUSTION IN CHP MICROTURBINES

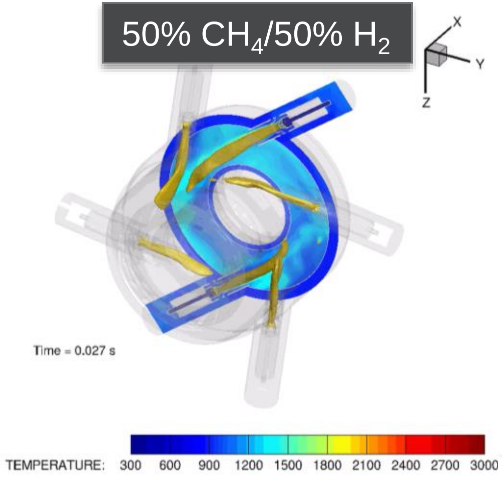
Impact of H_2 on flame shape and stabilization

- Unsteady RANS CFD calculations were performed to identify flame structure and onset of flashback.
- Simulations showed that stock hardware could sustain flashback-free combustion up to 75% H_2.
- Experimental investigations corroborated the simulation predictions.

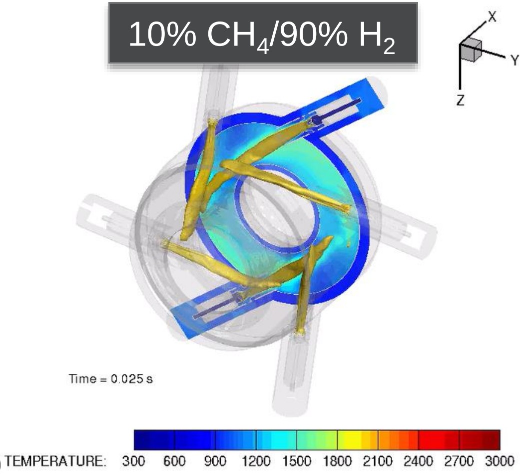


Temperature contour for a non-flashback condition/fuel blend

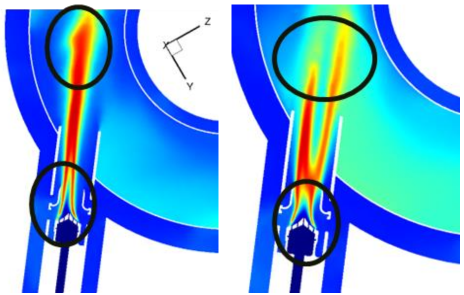
50% CH_4/50% H_2



10% CH_4/90% H_2



- Impact of flame stabilization on:
  - Combustion efficiency
  - Emissions (NOx, CO)



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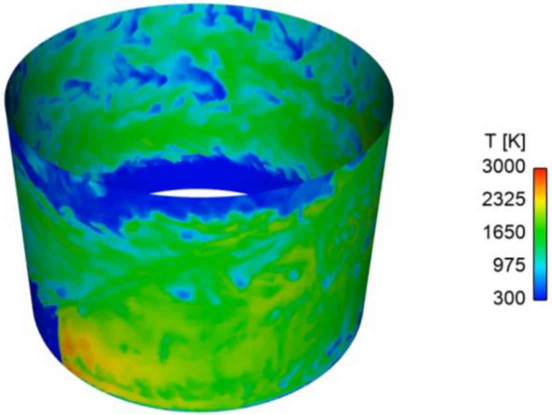
H_2 ROTATING DETONATION ENGINES (RDEs)

Benefits, Applications, and Challenges

- Faster and more intense heat release, decreased entropy generation, more available work and thermal efficiency than deflagrative combustion.
- Steady source of thrust. Compact design with no moving parts.
- Well-suited for hypersonic aircraft/rocket propulsion as well as stationary power generation.
- Multiple operating/design variables; complex design optimization difficult to handle with experiments alone.

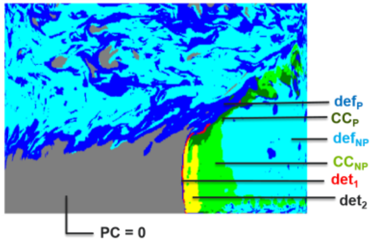


Challenges associated with RDE modeling:

- ❖ **High CFD simulation cost and runtime:** Need to capture detonation/shock fronts and account for full-scale RDE geometry and detailed chemistry; *O*(100M) cells; comprehensive parametric analysis becomes prohibitive.
- ❖ **Analysis/quantification of non-ideal combustion:** Lack of automated diagnostic tools that can be applied to large RDE simulation datasets to analyze and quantify non-ideal deflagrative losses.

Argonne's model development:

- Predictive/efficient LES/URANS for full-scale RDEs using AMR.
- Combustion diagnostic tool based on CEMA to quantify non-ideal losses.
- Successfully applied to a variety of fuels (Hydrogen, ethylene, methane).



CB: contact burning
PC: parasitic combustion
CC: commensal combustion

Combustion type	Fraction of total heat release (%)
def_P (predominantly contact burning (CB))	8.92
def_{NP}	5.06
det_1	29.94
det_2	47.26
CC_P	4.15
CC_{NP}	4.67

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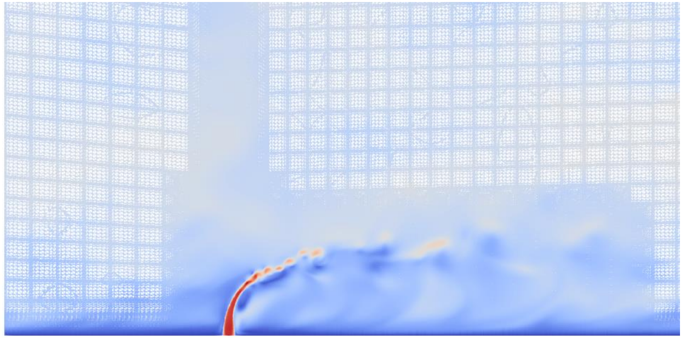
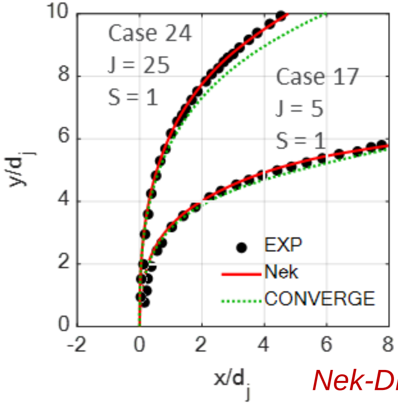
DNS OF H_2 JETS IN A CROSSFLOW

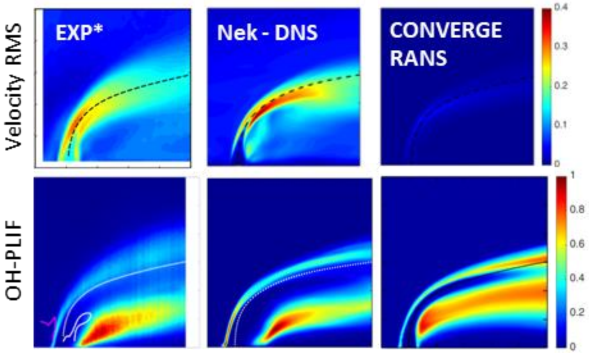


Polynomial order of 8, 91M grid points

Jet trajectory

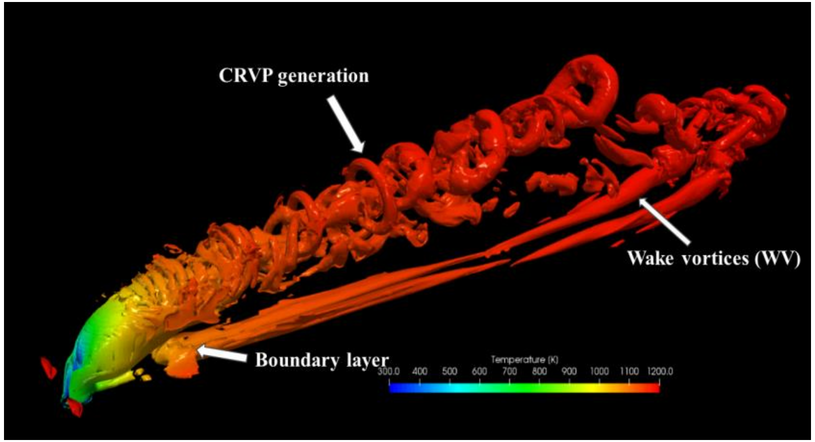


Flow and flame structures



Nek-DNS vs. CONVERGE-RANS

- Application to propulsion systems such as GTs, scramjets, and rockets.
- Simulation validated against experimental data from Georgia Tech JICF facility.
- Nek DNS reveal unsteady vortex structures, typically not captured using lower order numerics (e.g., RANS).
- High-order code better predicts mean jet trajectories, velocity RMS, and flame structures.



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THANK YOU FOR YOUR KIND ATTENTION! ANY QUESTIONS?

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