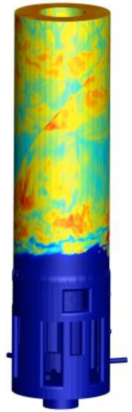
2024 UTSR & Advanced Turbines Program Review Meeting
September 25th, 2024

Physics Exploration and Analysis of Hydrogen-fueled Rotating Detonation Engines using Advanced Turbulent Combustion Modeling & High-fidelity Simulation Tools



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Research & Innovation Center
Donald Ferguson
Peter Strakey

Argonne LCRC

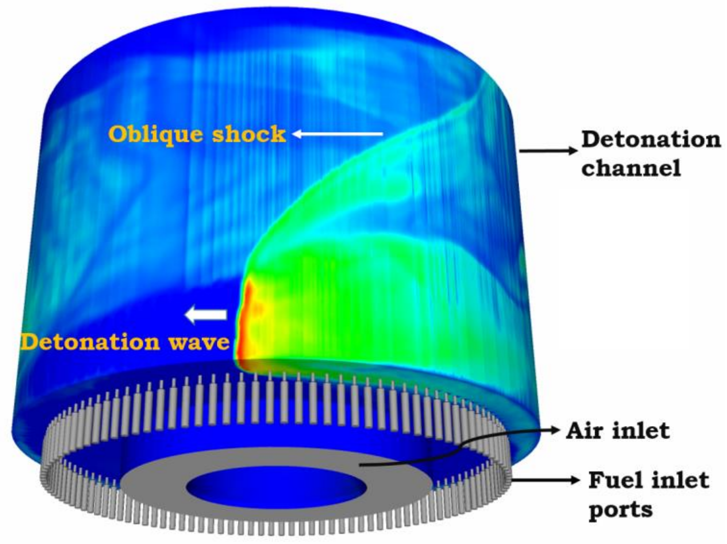
CONVERGENT SCIENCE

CFD software licenses

ROTATING DETONATION ENGINE (RDE)

What does it have to offer ?

- Detonation-based power cycles result in a ***pressure gain*** as reactants are converted to products
- Faster and more intense heat release, decreased entropy generation, more available work and thermal efficiency than deflagrative combustion
- **RDEs offer:**
  - ✓ *Steady source of thrust*
  - ✓ *High frequency: 100s to 1000s of Hz*
  - ✓ *Compact design with no moving parts*
  - ✓ *Well-suited for operation with hydrogen fuel for stationary power generation applications*



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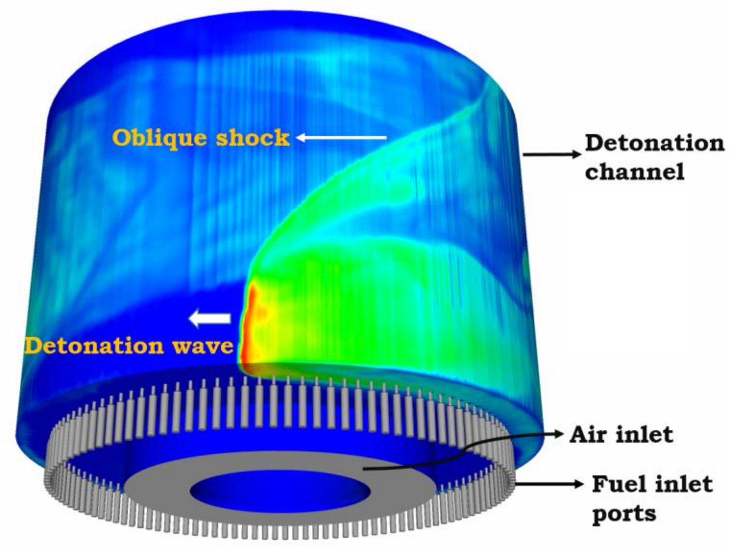
ROTATING DETONATION ENGINE (RDE)

Practical operability aspects

- A multitude of factors affect the performance of RDEs:
  - fuel and oxidizer compositions
  - global equivalence ratio
  - fuel/air mass flow rates
  - stagnation and back pressures
  - injector geometry/configuration
  - detonation channel geometry
  - RDC-inlet and RDC-turbine interactions



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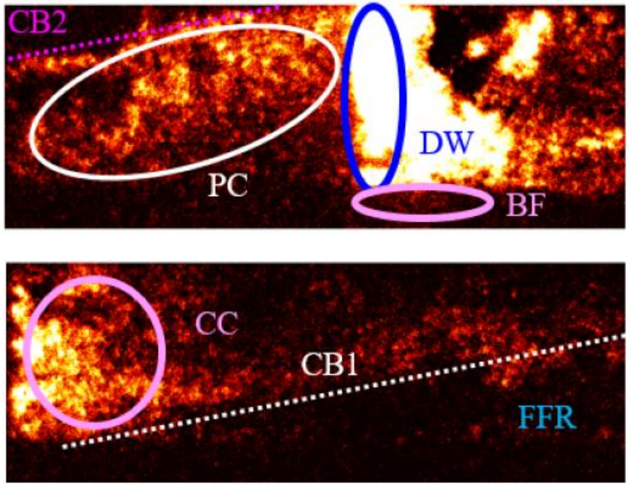
- Practical non-premixed RDE operation exhibits non-ideal deflagrative combustion phenomena; a mechanism of pressure loss



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

Chacon & Gamba, AIAA SciTech 2019

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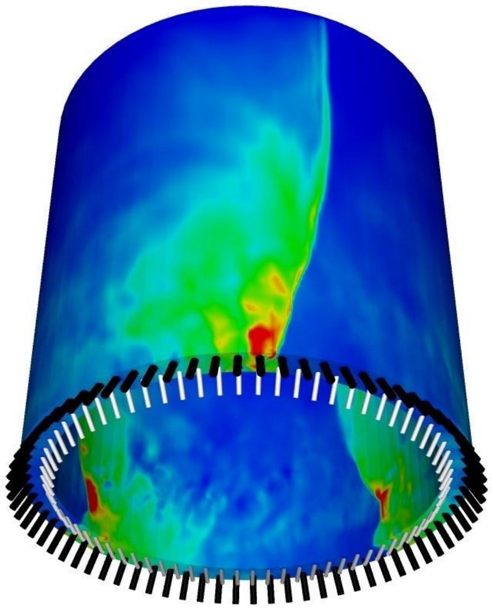
- Interaction of detonation wave(s) with wall boundary layers impacts wall heat transfer; relevant to RDE thermal management



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ROTATING DETONATION ENGINE (RDE)

CFD modeling challenges

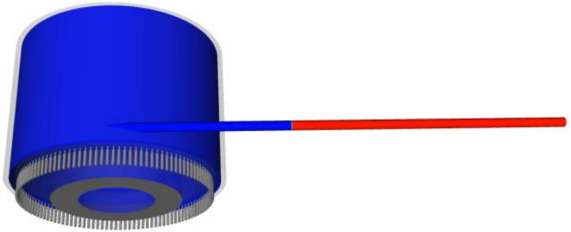
- Predictive and computationally efficient numerical modeling can complement experiments, and guide the development of practical RDE-based PGC systems

- However, multiple challenges exist for RDE CFD modeling:

➢ Expensive to incorporate *detailed (& stiff) fuel chemistry* in large-domain CFD simulations with (~10-100M) grid points

➢ Typical finite-rate chemistry (FRC) models do not account for *turbulence-chemistry interaction (TCI)* effects that can impact the CFD model capability to predict deflagrative losses

➢ *Detonation-boundary layer interactions* are not well studied due to high cost of wall-resolved simulations; subgrid wall models used in coarse-grained CFD are not well-validated for RDE-like conditions



$$\rho \frac{DY_k}{Dt} = -\nabla \cdot \mathbf{j}_k + \dot{\omega}_k$$

for $k = 1,2,\ldots,N_{species}$

PROJECT OVERVIEW

Overarching goals

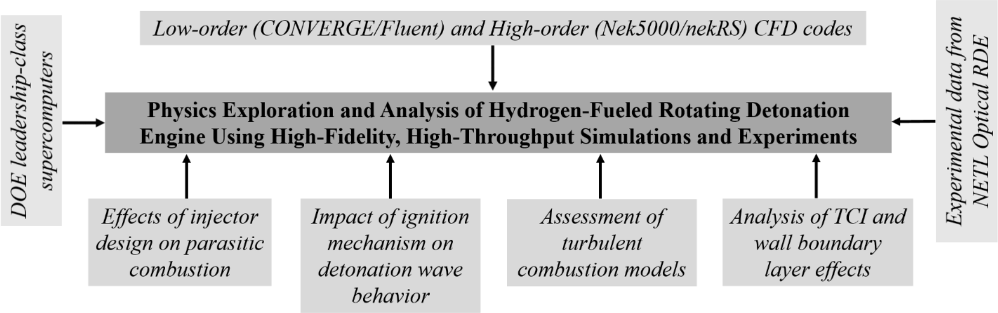
- Advance/accelerate predictive RDE CFD tools
- Leverage Argonne-NETL team's unique computational/experimental capabilities and leadership-class supercomputing for physics exploration and analysis of hydrogen RDEs
- Project Tasks:

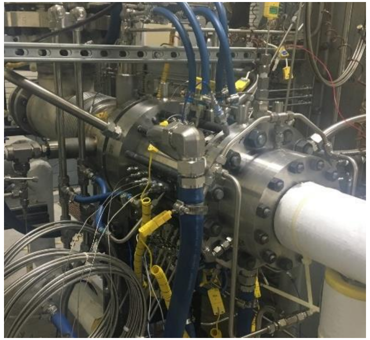
TASK 1: Reduced-order turbulent combustion models for predictive and computationally-efficient CFD simulations of full-scale RDEs

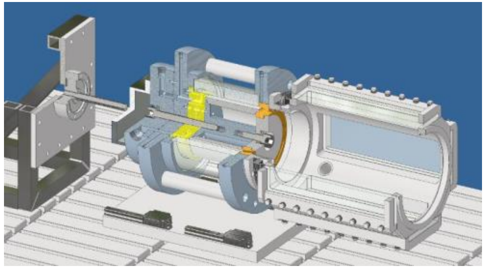
TASK 2: Scale-resolving simulations of RDE-relevant configurations to investigate TCI and wall boundary layer effects; improve turbulent combustion and wall models

TASK 3: Analysis of the effects of injector design on non-ideal parasitic losses in RDEs

TASK 4: Understanding the impact of ignition mechanism and initial transients on the quasi-steady behavior in RDEs







Test configuration: NETL water-cooled H_2-air RDE rig

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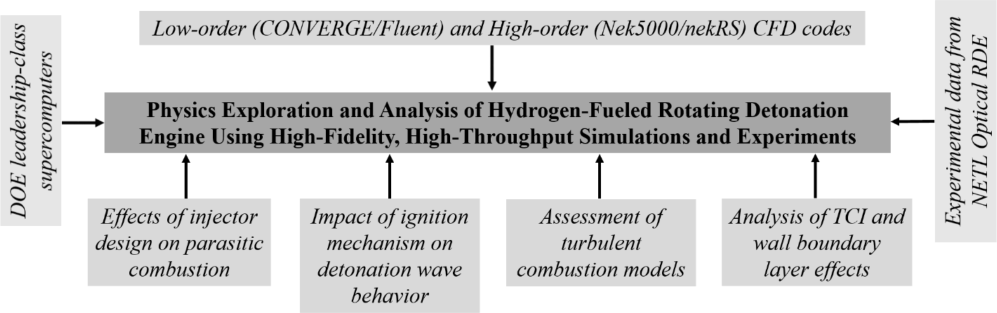
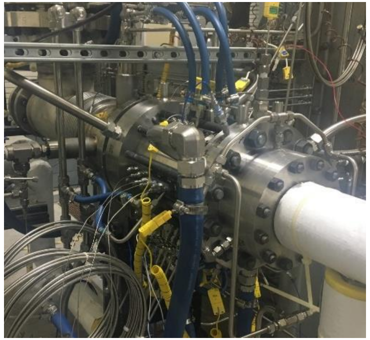
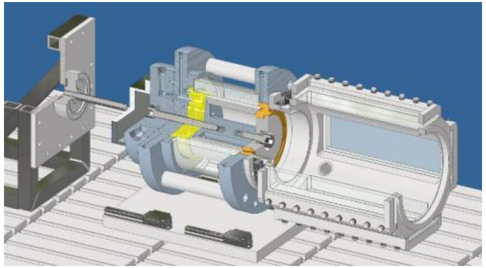






Test configuration: NETL water-cooled H_2-air RDE rig

Demir et al., AIAA-2022-2073

Kabil and Xu, AIAA-2023-0160

TASK 1a

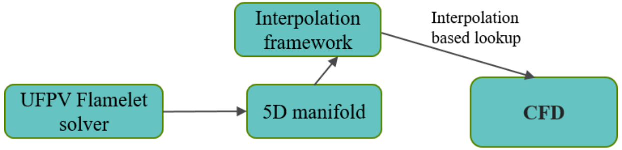
Turbulent combustion modeling for predictive and efficient RDE CFD simulations

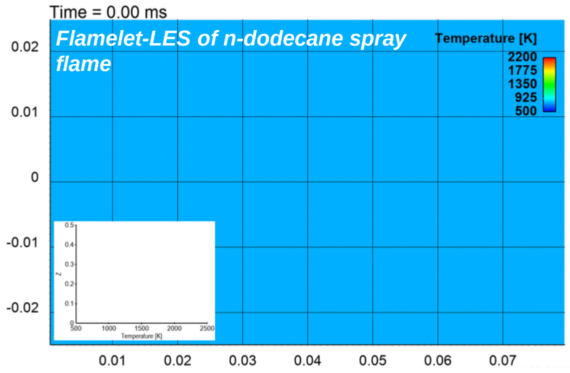
- Argonne's in-house **compressible Unsteady Flamelet Progress Variable (UFPV) model** captures turbulent non-premixed combustion with subgrid TCI effects
- Reduced-order representation of thermochemical state as a function of a few conditioning variables (*Z*, Z_{var}, *C, P, etc.)* as a look-up table → *achieves speedup over FRC approach via reduction in the number of transport equations and associated chemical stiffness*
- Previously demonstrated for spray flames, jet-in-crossflow (JICF), IC engine, and scramjet engine CFD simulations
- **Goal:** Adapt the UFPV modeling framework for premixed/partially-premixed RDE-like conditions and demonstrate in RDE large-eddy simulations (LES)
- Predictive accuracy and simulation speedup will be benchmarked against the baseline FRC approach and NETL RDE experimental data

$$\frac{\partial(\bar{\rho}\tilde{Z})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{Z})}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t}\right)\frac{\partial\tilde{Z}}{\partial x_i}\right]$$

$$\frac{\partial(\bar{\rho}\widetilde{Z''^2})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\widetilde{Z''^2})}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t}\right)\frac{\partial\widetilde{Z''^2}}{\partial x_i}\right] + 2\frac{\mu_t}{Sc_t}\left(\frac{\partial\tilde{Z}}{\partial x_i}\right)^2 - \bar{\rho}\tilde{\chi}$$

$$\frac{\partial(\bar{\rho}\tilde{C})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{C})}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t}\right)\frac{\partial\tilde{C}}{\partial x_i}\right] + \tilde{\dot{\omega}}_c$$





TASK 1b

Turbulent combustion modeling for predictive and efficient RDE CFD simulations

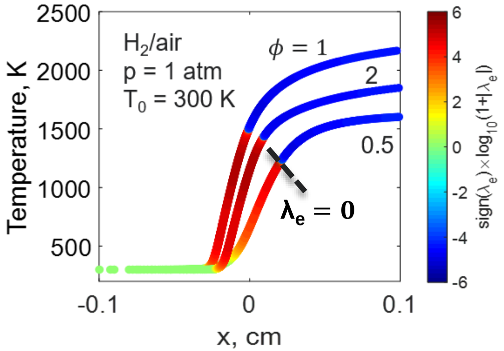
- **Chemical explosive mode analysis (CEMA)** based framework developed for <u>advanced flame diagnostics and multi-regime turbulent combustion modeling</u>
  - Identifies local combustion modes in the reacting flow-field based on eigen-analysis of the Chemical Jacobian
  - Suitable combustion models can be locally assigned on-the-fly in a regime-adaptive fashion
  - Accelerates simulations compared to FRC approach while preserving accuracy
- **Goal:** Demonstrate CEMA-aided regime-adaptive combustion model and compare against monolithic FRC and UFPV models for RDE-LES

Lu *et al.*, JFM 2010

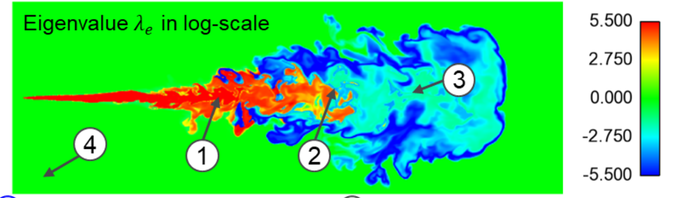
$$\frac{D\boldsymbol{y}}{Dt} = \boldsymbol{g}(\boldsymbol{y}) = \boldsymbol{\omega}(\boldsymbol{y}) + \boldsymbol{s}(\boldsymbol{y})$$

$$\mathbf{J}_\omega = \frac{\partial \boldsymbol{\omega}}{\partial \mathbf{y}}$$

$$\lambda_e = \boldsymbol{b} \cdot \mathbf{J}_\omega \cdot \boldsymbol{a}$$

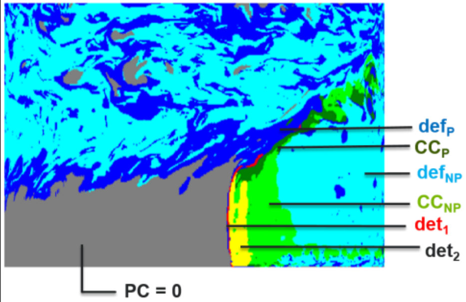


Modeling of turbulent partially premixed flames[3]



1. Non-premixed flamelets for post-ignition zone: $\lambda_e < -1$
2. Thicken flame model for premixed fronts: $\lambda_e = 0$
3. Finite rate chemistry for pre-ignition zone: $\lambda_e > 1$
4. Inert mixing for chemically inactive zone: $|\lambda_e| < 1$

Combustion regime analysis of RDEs[1,2]



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

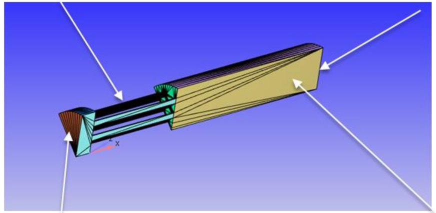
[1]Pal *et al.*, AIAA-2020-2161
[2]Pal *et al.*, AIAA-2020-3086
[3]Xu *et al.*, CNF 2018

TASK 1a PROGRESS UPDATE

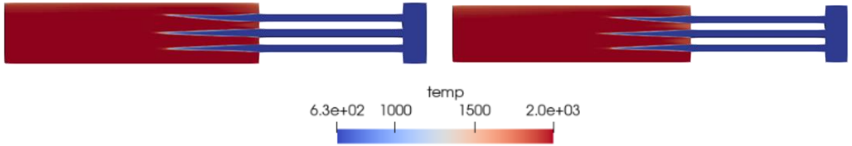
UFPV model adaptation for premixed/partially-premixed flames

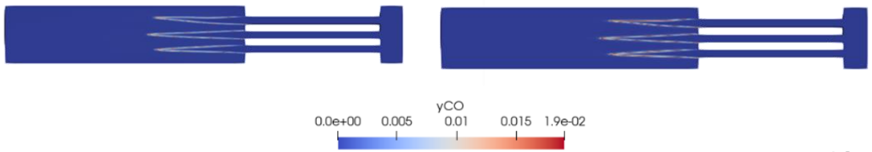
- Premixed UFPV look-up tables were generated based on freely propagating 1D premixed flames (instead of counterflow non-premixed flames)
- The UFPV model was coupled with CONVERGE CFD solver
- Preliminary RANS demonstration studies were performed for verification and validation of the premixed UFPV implementation

Premixed methane-air model combustor

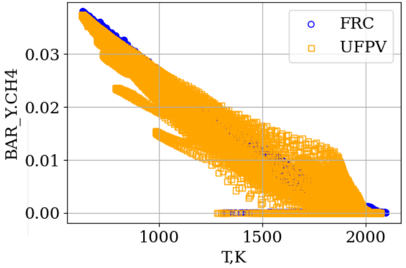


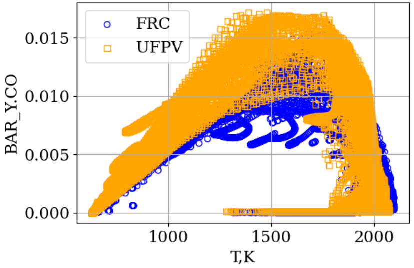
FRC **UFPV**





Statistically steady state





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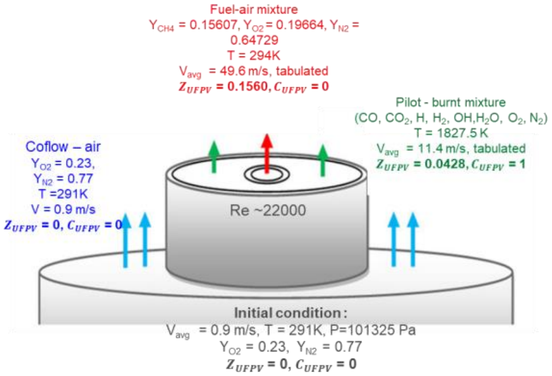
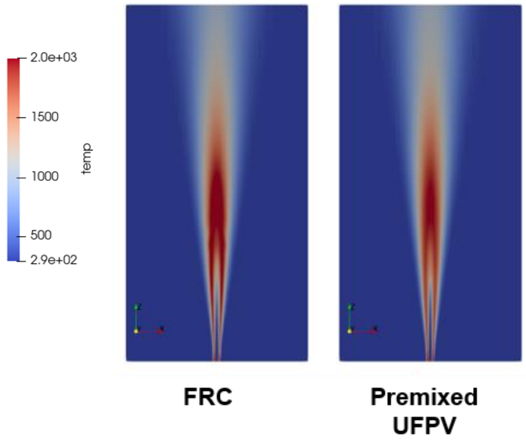
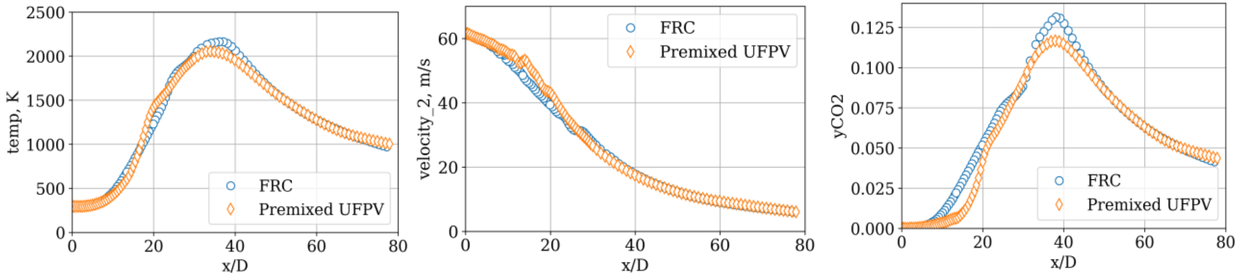
Piloted partially-premixed methane-air flame (Sandia Flame D)





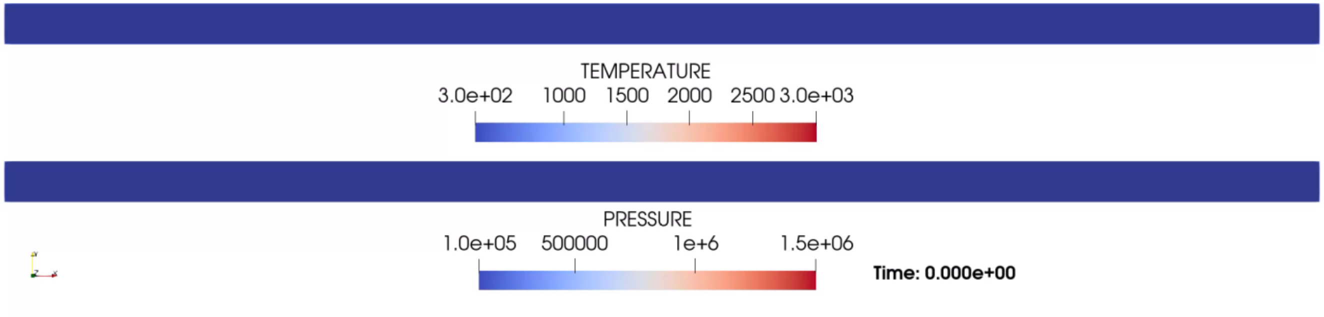
Centerline profiles



TASK 1a PROGRESS UPDATE

Ongoing/Future work

- Extension of premixed UFPV modeling framework to detonations and demonstration for fully-premixed detonation tube simulations is currently underway
- Afterwards, the extended UFPV model will be applied to practical RDE configurations



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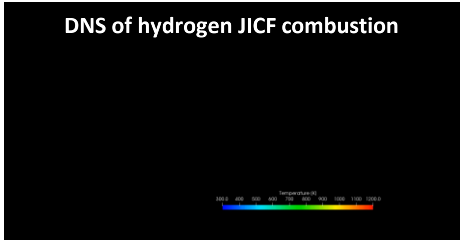
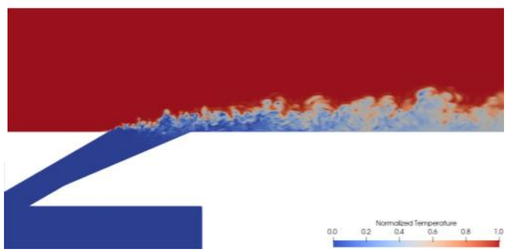
Wu et al., AIAA-2023-1641
Xu et al., AIAA-2022-0823
Nunno et al., AIAA-2022-1404

TASK 2

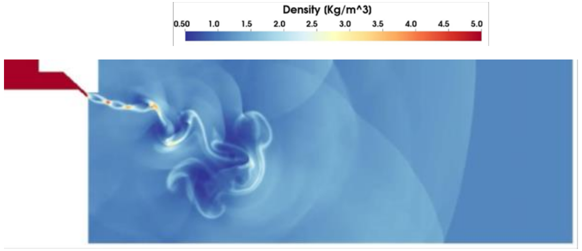
Scale-resolving simulations using high-order Nek5000 CFD solver



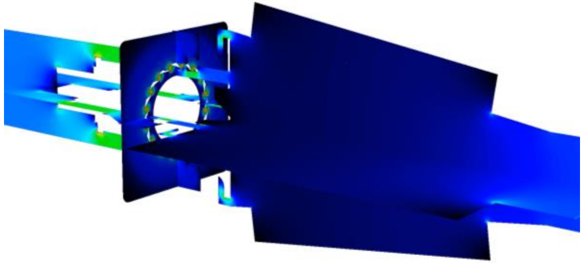
- High-order spectral element method (SEM) formulation in Argonne's Nek5000 solver
  - Solution is represented as N^{th} order tensor-product polynomials (N ~ 5-15)
  - Exponential (spectral) convergence with N
  - Discontinuous Galerkin version to handle compressible flows with shock waves
- Capability to handle complex/realistic engine geometries (struc./unstruc. meshes)
- Demonstrated scalability on leadership-class DOE supercomputers
- Extensively used for high-fidelity simulations of compressible non-reacting & low-mach/incompressible reacting/non-reacting flows relevant to gas turbines and piston engines
- **Goal:** Leverage Nek5000 to perform DNS/WRLES of RDE-relevant configurations to investigate TCI and wall boundary layer effects; utilize high-fidelity datasets to improve turbulent combustion and subgrid wall models



WRLES of Gas Turbine Film Cooling



2D DNS of Hydrogen DI Under-expanded Jets



ARC-M1 combustor: High-fidelity WRLES using Nek5000

Keeton et al., APS-DFD 2024

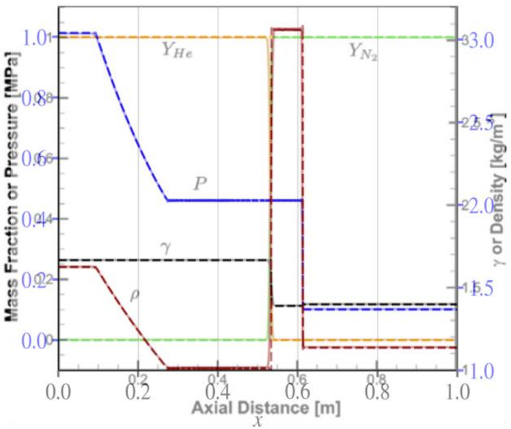
Keeton et al., AIAA SciTech 2025 (accepted)

TASK 2 PROGRESS UPDATE

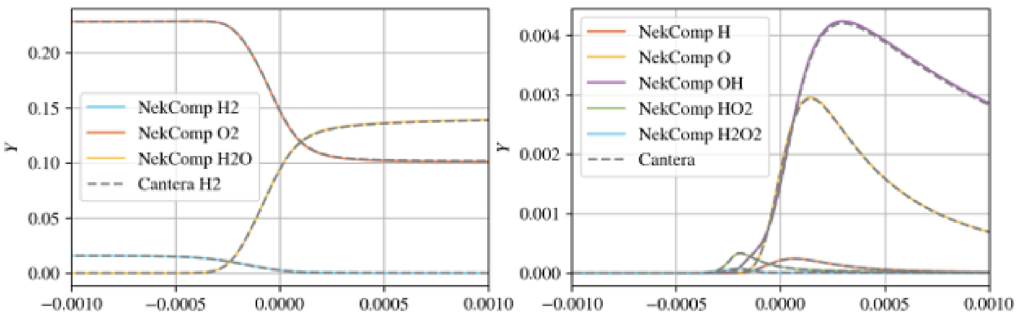
Compressible reacting Nek5000 solver development

- Solves for chemically reacting compressible Navier-Stokes equations
- Fully-conservative Discontinuous Galerkin (DG) SEM with artificial viscosity to stabilize the solution near flow discontinuities (shocks)
- Thermodynamic/transport properties and reaction rates computed using Cantera
- Positivity-preserving limiters to enforce non-negative energy and species concentrations
- Operator splitting schemes to separately solve for convection-diffusion and reaction

1D multicomponent shock tube



1D laminar premixed flame

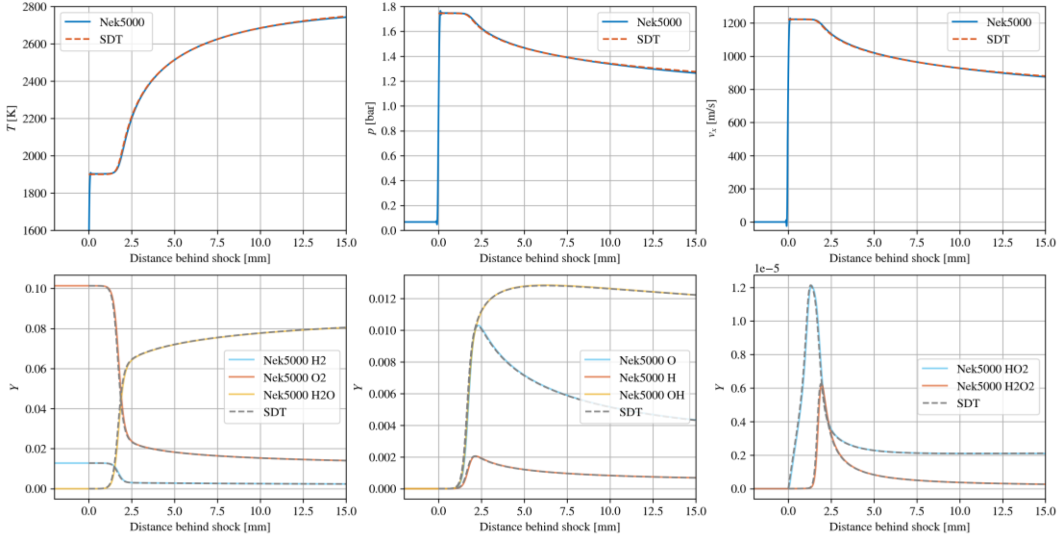


TASK 2 PROGRESS UPDATE

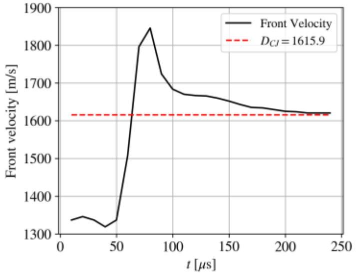
Compressible reacting Nek5000 solver demonstration for detonations

1D detonation setup

- 1D Euler
- $x \in [0, 0.45]$ m
- $h = 90\ \mu m$
- Polynomial order, $N = 3$
- $H_2/O_2/Ar$ detailed chemistry
- $P_0 = 0.0667$ bar
- $T_0 = 298$ K
- $X_{H_2} : X_{O_2} : X_{Ar} = 2 : 1 : 7$



	T_{vN} [K]	p_{vN} [kPa]
SDT	1899.9	174.5
Nek5000	1902.4	174.6



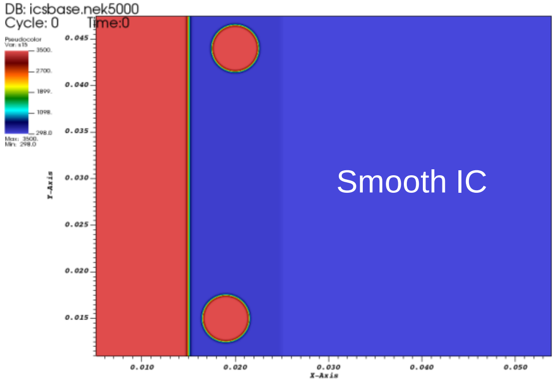
Keeton et al., APS-DFD 2024
Keeton et al., AIAA SciTech 2025 (accepted)

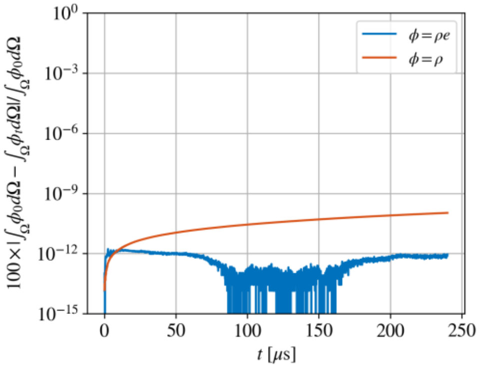
TASK 2 PROGRESS UPDATE

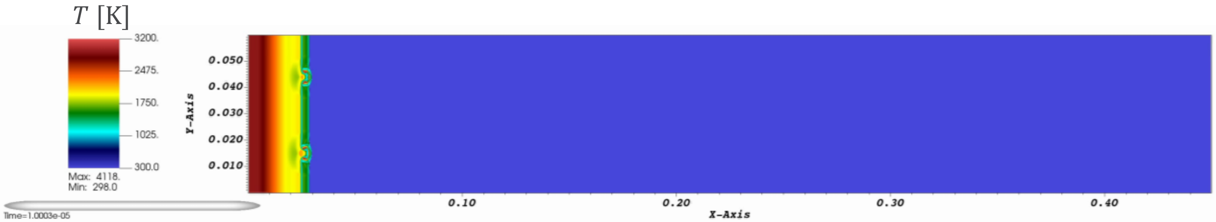
Compressible reacting Nek5000 solver demonstration for detonations

2D detonation setup

- 2D Euler
- $x \in [0,0.45]$ m
- $y \in [0,0.06]$ m
- $h = 90\ \mu m$
- Polynomial order, $N = 2$
- $E = 3.34\text{M}$
- Grid points $= 30\text{M}$
- $H_2/O_2/Ar$ detailed chemistry
- $P_0 = 0.0667$ bar
- $T_0 = 298$ K
- $X_{H_2}:X_{O_2}:X_{Ar} = 2:1:7$







- **Future work:** Detonation propagation in stratified mixtures; turbulent fluctuations; investigate TCI effects

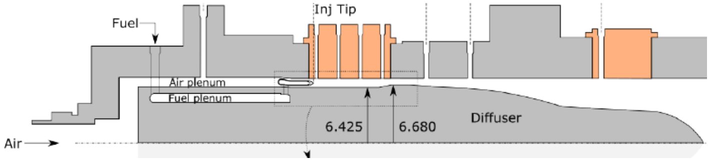
FULL-SCALE RDE SIMULATIONS

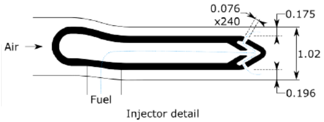
NETL-RDE LES modeling with finite-rate chemistry

- Wall-modeled large-eddy simulation (WMLES) framework developed in CONVERGE
- Detailed hydrogen/air chemistry 9 species and 21 reactions (O'Conaire *et al.* 2004)
- Adaptive mesh refinement (AMR) based on velocity, temperature, and pressure for trade-off between accuracy and computation time
- Preliminary model validation was performed against NETL experimental data

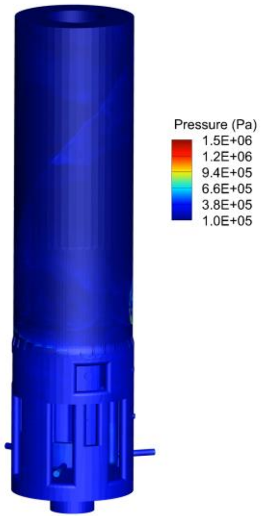
Case #	Air mass flow rate (kg/s)	Fuel mass flow rate (kg/s)	Global equivalence ratio	T_{air} (K)	T_{fuel} (K)	P_{back} (kPa)	Expt. wave speed (m/s)	CFD wave speed (m/s)
1	0.5621	0.01191	0.725	431	331	133	1615	1670 ± 20
2	0.5218	0.01362	0.894	432	330	131	1600	1750 ± 15

- The LES-FRC model will be utilized for Tasks 1-4





Pintle injector



THANK YOU

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