# 2023 INCITE Proposal Submission
## Proposal

**Title: DNS and LES of Gas Turbine Combustors for Sustainable Aviation Fuels**
**Principal Investigator: Muhsin Ameen**
**Organization: Argonne National Laboratory**
**Date/Time Generated: 6/17/2022 4:26:36 PM**

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# Section 1: PI and Co-PI Information

### Question #1

***Principal Investigator:*** *The PI is responsible for the project and managing any resources awarded to the project.  If your project has multiple investigators, list the PI in this section and add any Co-PIs in the following section.*

### Principal Investigator


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**Question #2**

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**Question #3**

***Institutional Contact:*** *For the PI's institution on the proposal, identify the agent who has the authority to review, negotiate, and sign the user agreement on behalf of that institution. The person who can commit an organization may be someone in the contracts or procurement department, legal, or if a university, the department head or Sponsored Research Office or Grants Department.*

**Institutional Contact**

**Institutional Contact Name**

Jacki Flood

**Institutional Contact Phone**

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# Section 2: Project Information

**Question #1**

*Select the category that best describes your project.*

**Research Category**

Energy Technologies: Energy Efficiency

**Question #2**

*Please provide a project summary in two sentences that can be used to describe the impact of your project to the public (50 words maximum)*

**Project Summary**

Sustainable aviation fuels or SAFs have gained popularity as a means to achieve zero-carbon aviation by 2050. High-fidelity device-level simulations using Nek5000 will provide fundamental insights into the effect of fuel behavior on the combustion dynamics in gas turbine combustors and enable engine design changes for transitioning to SAFs.

# Section 3: Early Career Track

**Question #1**

***Early Career***

*Starting in the INCITE 2022 year, INCITE is committing 10% of allocatable time to an [Early Career Track](#) in INCITE. The goal of the early career track is to encourage the next generation of high-performance computing researchers. Researchers within 10 years from earning their PhD (after December 31st 2012) may choose to apply. Projects will go through the regular INCITE Computational Readiness and Peer Review process, but the INCITE Management Committee will consider meritorious projects in the Early Career Track separately.*

***Who Can Apply**: Researchers less than 10 years out from their PhD that need LCF-level capabilities to advance their overall research plan and who have not been a previous INCITE PI.*

***How to Apply:***

*In the regular application process, there will be a check-box to self-identify as early career.*

- *The required CV should make eligibility clear.*
- *If awarded, how will this allocation fit into your overall research plan for the next 5 years?*

*Projects will go through the regular INCITE review process. The INCITE Program is targeting at least 10% of allocatable time. When selecting the INCITE Career Track, PIs are not restricted to just competing in that track.*

- *What is the Early Career Track?*
    - *The INCITE Program created the Early Career Track to encourage researchers establishing their research careers. INCITE will award at least 10% of allocatable time to meritorious projects.*
- *Will this increase my chances of receiving an award?*
    - *Potentially, this could increase chances of an award. Projects must still be deemed scientifically meritorious through the review process INCITE uses each year.*
- *What do I need to do to be considered on the Early Career Track?*
    - *In the application process, select 'Yes' at 'If you are within 10 years of your PhD, would you like to be considered in the Early Career Track?' You will need to write a paragraph about how the INCITE proposal fits into your 5-year research and career goals.*

- *What review criteria will be used for the Early Career Track?*
    - *The same criteria for computational readiness and scientific merit will be applied to projects in the Early Career Track as will be applied to projects in the traditional track. The different will be manifest in awards decisions by the INCITE management committee.*

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**Early Career Track**

**If you are within 10 years of your PhD, would you like to be considered in the Early Career Track? Choosing this does not reduce your chances of receiving an award.**

Yes

**If ‘yes’, what year was your PhD? If 'no' enter N/A**

2014

**If ‘yes’, how will this allocation fit into your overall research plan for the next 5 years? If 'no' enter N/A.**

I am currently a senior research scientist in the Center for Advanced Propulsion and Power Systems at Argonne National Laboratory. I have more than 10 years of experience in high performance computing, high-fidelity simulations, and turbulent combustion modeling. He has significant expertise in using Nek5000 for performing high-fidelity device-level simulations on leadership-class supercomputers. He has previously served as the PI on an ALCC 2019 allocation, a co-PI on an INCITE 2021 allocation and PI on multiple DD allocations. My current role at the center is to lead the development and use of massively parallel CFD codes (such as Nek5000 and NekRS) for applications relevant to transportation and power generation. This also involves reaching out to industry partners to try to align the research goals with the short- and long-term needs of the transportation and power generation industries.

From 2018-2021, I was a PI on PACE, a multi-lab project funded by DOE’s Vehicle Technologies Office (VTO), with the goal of developing fast and accurate submodels for internal combustion engines. As part of this project, my team was leading the development and use of Nek5000 to perform direct numerical and large eddy simulations of internal combustion engines. We heavily leveraged supercomputing resources through multiple DD, ALCC, and INCITE allocations to meet the project milestones. With the current administration’s focus on decarbonization, the light- and medium-duty on-road transportation systems are set to be electrified. However, there is a pressing need to decarbonize the hard-to-electrify sectors such as aviation. Sustainable aviation fuels or SAFs have gained popularity as a means to achieve net zero-carbon aviation by 2050. SAF is a clean substitute for fossil-based jet fuel and is produced from sustainable resources such as biomass. Realizing the importance of high-fidelity simulations to support this effort, VTO has provided a pilot funding for my team to transfer the expertise and learnings from the PACE program to modeling gas turbine combustors operating on

SAFs. The objective of this pilot project is use Nek5000 simulations to identify and understand the effect of properties of SAF on the gas turbine combustion dynamics. If we are able to show early successes, there is a huge potential for this pilot project to expand to a larger project. Based on the scale of the challenges, I envision the establishment of a multi-lab project, involving multiple experimental and simulation teams, with industry supervision with a duration of more than 5 years. Having access to an INCITE allocation will help kickstart the role of my team in helping the aviation sector make a quick transition to SAFs.

Following the completion of the INCITE award, the datasets generated from this allocation will be utilized over the next 5 years to provide:
(1) An open-source repository for academic and industrial researchers for validation and verification against their models
(2) Improved combustion and heat transfer models suitable for SAFs. These models could be ported into existing engineering-level codes used by industry to accelerate the design process for engines.
(3) Improved correlations between the turbulent flow structures, fuel properties, and combustion dynamics leading to an improved understanding of the sensitivity of the combustor performance to SAF fuel properties.

Ultimately, I believe these efforts will influence technology development for engines and fuels leading to deep decarbonization by 2050.

# Section 4: INCITE Allocation Request & Other Project Funding/Computing Resources

**Question #1**

**OLCF Summit (IBM / AC922) Resource Request - 2023**

**Question #2**

**OLCF Frontier (Cray Shasta) Resource Request – 2023**

**Question #3**

**OLCF Frontier (Cray Shasta) Resource Request – 2024**

**Question #4**

**OLCF Frontier (Cray Shasta) Resource Request – 2025**

**Question #5**

**ALCF Theta (Cray XC40) Resource Request - 2023**

**Node Hours**

2.46 Million

**Storage (TB)**

166

**Off-Line Storage (TB)**

180

**Question #6**

**ALCF Polaris Resource Request - 2023**

**Question #7**

**ALCF Polaris Resource Request - 2024**

**Question #8**

**ALCF Polaris Resource Request - 2025**

**Question #9**

**ALCF Aurora (Intel $X^e$) Resource Request – 2023**

**Question #10**

**ALCF Aurora (Intel $X^e$) Resource Request – 2024**

**Question #11**

**ALCF Aurora (Intel $X^e$) Resource Request – 2025**

**Question #12**

*List any funding this project receives from other funding agencies.*

**Funding Sources**

**Funding Source**

US Department of Energy (DOE) Vehicle Technologies Office (VTO)

**Grant Number**

VT1602000-05450-1005769

**Question #13**

*List any other high-performance computing allocations being received in support of this project.*

**Other High Performance Computing Resource Allocations**

# Section 5: Project Narrative and Supplemental Materials

**Question #1**

*Using the templates provided here, please follow the [INCITE Proposal Preparation Instructions](#) to prepare your proposal. Elements needed include (1) Project Executive Summary, (2) Project Narrative, (3) Personnel Justification and Management Plan, (4) Milestone Table, (5) Publications Resulting from prior INCITE Awards (if appropriate), and (6) Biographical Sketches for the PI and all co-PI's. Concatenate all materials into a single PDF file. Prior to submission, it is strongly recommended that proposers review their proposals to ensure they comply with the proposal preparation instructions.*

**Concatenate all materials below into a single PDF file.**

1. **Project Executive Summary (One Page Max)**
2. **Project Narrative (15 Pages Max)**
3. **Personnel Justification and Management Plan (1 Page Max)**
4. **Milestone Table**
5. **Publications resulting from prior INCITE Awards (if appropriate)**
6. **Biographical Sketches for the PI and all co-PI's.**

2023_INCITE_Concatenated_AmeenDasguptaWu.pdf
The attachment is on the following page.

## PROJECT EXECUTIVE SUMMARY

**Title:** DNS and LES of Gas Turbine Combustors for Sustainable Aviation Fuels

**PI and Co-PI(s):** Muhsin Ameen (PI), Debolina Dasgupta (co-PI), Sicong Wu (co-PI)

**Applying Institution/Organization:** Argonne National Laboratory

**Resource Name(s) and Number of Node Hours Requested:** 2.46M node-hours on ALCF Theta

**Amount of Storage Requested:** 166 TB on ALCF Theta

**Executive Summary:**

With a push towards decarbonization, Sustainable Aviation Fuels (SAFs) have grown to prominence as a means for the aviation sector to reduce its carbon footprint. The chemical compositions of SAFs are different from conventional jet fuels leading to variations in physical and chemical properties. The flow within gas turbines is highly turbulent and complex due to multiple air streams and swirling flow resulting in flow features such as recirculation zone and shear layers. The combination of the flow features and the different fuel properties result in a varied distribution of liquid and vaporized fuel within the combustor resulting in different flame stabilization, shape, and structure. The behavior of the stable flame is also a strong indicator of the fuel's response to off-normal operations such as lean blow out, cold start, and high-altitude relight. The aim of this INCITE proposal is to develop a detailed understanding of the impact of the fuel and flow on the flame dynamics using a combination of Large-Eddy Simulations (LES) and Direct Numerical Simulations (DNS), with a specific focus on SAFs. The high-fidelity LES will provide and understanding on the impact of flame shape, flame anchoring and flow features, and the DNS will provide unprecedented details of the change in flame structure and provide data to improve combustion models further for partially premixed flames. Nek5000, which is a leading high-order spectral element, open-source code for accurate modeling of fluid turbulence, will be used in the current project to perform these simulations.

Wall-resolved LES will be performed for a realistic gas turbine combustor, the midsize Army Research Combustor (ARC-M1). High-fidelity simulations of such a complex gas turbine combustor using high-order codes are highly unique. Using a 128K node-hour DD allocation on ALCF Theta, non-reacting flow for this combustor has been simulated. These simulations demonstrated the capability of the modeling framework to capture the flow features in such devices. The proposal leverages capabilities developed through this allocation and under large DOE programs like the Exascale Computing Project (ECP) to perform first-of-its-kind calculations of multi-physics and multiscale liquid fuel turbulent reacting flows in gas turbine engines.

The proposed project includes three tasks. The first task consists of performing wall-resolved LES of the ARC-M1 combustor using conventional jet fuel (A-2). To understand the impact of flow features, a detailed analysis of the liquid fuel, vaporized fuel, flame shape, flame anchoring, flame area will be performed. In addition, to understand the coupling between the non-reacting and reacting flow with the spray, dominant energy modes and associated structures will be identified. The second task involves performing wall-resolved LES of the ARC-M1 combustor using a SAF surrogate. A similar analysis as the previous task will be performed to contrast and compare the critical flow and flame dynamics changes due to changes in fuel properties. The third task involves DNS of a simplified swirl stabilized combustor. A total of four cases will be simulated using A-2 and SAF for two operating conditions. Flame structure comparison using conditional means will be performed for both fuels to understand how and why varying fuel properties and air temperature changes the structure. This database of detailed flame structure can also be used for improving combustion models. Overall, the knowledge gained from this project will significantly improve our understanding of SAFs compared to conventional jet fuel. In addition, it will also aid in the development of tools that can be used for assessing other SAFs produced in the future.

**PROJECT NARRATIVE**

# 1 SIGNIFICANCE OF RESEARCH

## 1.1 Decarbonization of Aviation Using Sustainable Aviation Fuels

The transportation sector is the largest contributor to Green House Gas (GHG) emissions. In fact, it comprises about 27% of the GHG emissions [1] within the United States. Out of this 27%, aircraft emissions are the third largest contributor next to light, medium, and heavy-duty vehicles [1]. With a push towards electrification of light-duty and medium-duty vehicles, the percentage contribution from aviation is expected to be much higher. It is, thus, imperative to develop pathways for decarbonization of the aviation sector.

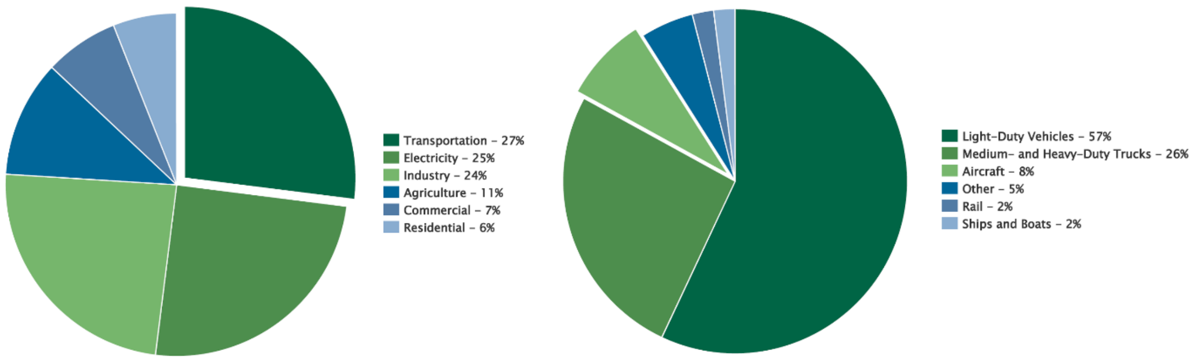


**Figure 1. 2020 U.S. GHG Emissions by Sector (left) and 2020 U.S. Transportation Sector GHG Emissions by Source [1]**

Sustainable aviation fuels or SAFs have gained popularity as a means to achieve net zero-carbon aviation by 2050 [2]. SAF is a clean substitute for fossil-based jet fuel and is produced from sustainable resources such as biomass. Depending on the feedstock and the pathways to produce the fuel, SAF can reduce life cycle GHG emissions dramatically compared to current jet fuels [2]. The White House has launched the SAF Grand Challenge to expand SAF production to ensure transition from conventional jet fuels to SAFs [3]. However, large-scale SAF production is only a part of solution of reducing emissions. It is important to assess how these fuels would perform in the current aircraft fleet, thus necessitating end-use research for these fuels.

Currently, two categories of SAFs exist namely "drop-in" fuels and "non-drop-in" fuels. Compositionally, drop-in fuels have slightly different fuel properties and compositions compared to petroleum jet fuel. They can be blended with conventional jet fuels at smaller percentages and can be used in today's aircraft engines without modification while providing the same level of performance and safety as today's petroleum-derived jet fuel. However, the fuel performance using 100% drop-in fuels is unknown. Additionally, with a push towards large-scale SAF production and adoption, more feedstock and pathways of SAF productions are currently being employed to produce non-drop-in SAFs. These non-drop-in fuels have different composition compared to jet fuels (for example, the percentages of normal and iso-alkanes, cycloparaffins, aromatics in the fuel blend). These differences in composition can lead to changes in the chemical and physical properties between conventional jet fuel and non-drop-in SAFs. In addition, the change in the composition will also influence the non-volatile particulate matter (nVPM) emissions that need to be reduced to ensure good air quality and to reduce contrail formation that can contribute to the global radiative forcing. Thus, there is a significant research opportunity in understanding the impact of the changes in the fuel properties of the SAFs on the flame and flow dynamics within the gas turbine combustors.

Gas turbines operate lean to ensure reduced NOx, CO, and unburnt hydrocarbon emissions. However, at these lean conditions, the combustors have limited margins between stable and unstable behavior. In typical swirl-stabilized gas turbine combustors, during stable operation, the hot products recirculate and aid in the heating, vaporizing, and subsequently ignition of the reactant mixture [4]. This is pictorially depicted in Figure 2. This behavior and structure of the stabilized flame is dependent on several factors such as quality of atomization, fuel vaporization, fuel/air mixing, chemical reaction rates etc.

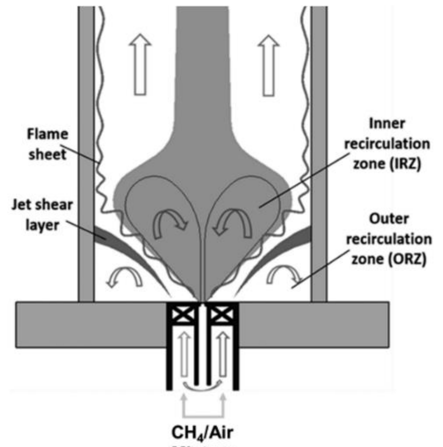


**Figure 2. Schematic illustrating the flow patterns within a swirl combustor [4]**

The performance of the fuel within the combustor is determined by three figures of merit identified as a part of the National Jet Fuel Combustion Program (NJFCP). These are lean blow out (LBO), High altitude relight and Cold Start. LBO occurs when the flame is advected out of the combustor if the flame speed cannot match the flow speed or the flame extinguishes due to the reduction in the heat released due to combustion [5]. An example of lean blow out in a realistic gas turbine combustor is shown in Figure 3 (left image). High-altitude relight re-establishes a flame within the combustor in the event of loss of flame and is usually characterized by low fuel and air temperatures and pressures. For cold start, while the pressure is higher, the fuel and air temperatures are low. In both cases, an igniter ignites the flow and the success is dependent on the ability of the ignition kernel to grow leading to fuel vaporization and subsequent ignition. A successful ignition event is shown in Figure 3 (right image). All three metrics are closely tied to the flame and flow dynamics within gas turbine combustors that influences the fuel's ability to ignite and form a stable flame. The internal dynamics within gas turbines is a fundamental problem of multi-scale, multi-physics interactions. The complex flow-field is highly turbulent and is responsible for the liquid spray formation and the spray droplet distribution [6, 7]. This results in a spatio-temporal variation of liquid and vaporized fuel-air mixture. This distribution impacts the flame shape, its stabilization and its response to the flow-field around it. Typically, partially premixed flames are formed within these combustors and this flame structure is also dependent on the fuel-air distribution [4]. For different fuels, the vaporization and distribution in the combustor can be significantly different resulting in large differences in combustion characteristics even at the same operating condition. As an example, Figure 4 shows the averaged flame shape for three fuels: A-2 (conventional jet fuel), C-1

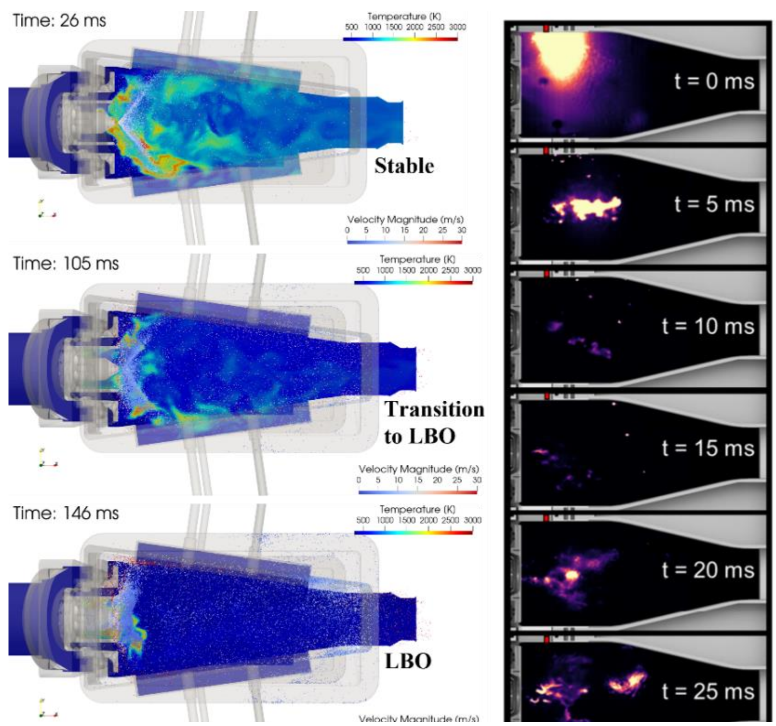


**Figure 3. (left) Lean blow out due to reduced heat release caused by a reduction of fuel flow rate from the stable condition, Center plane of combustor colored by temperature contours and spray droplets colored by velocity magnitude [6] (right) Time-series of broadband imaging of ignition [7]**

(a low cetane number fuel) and C-5 (flat boiling curve) for the same operating condition. A clear difference in flame shape, flame height and stabilization location are noted.

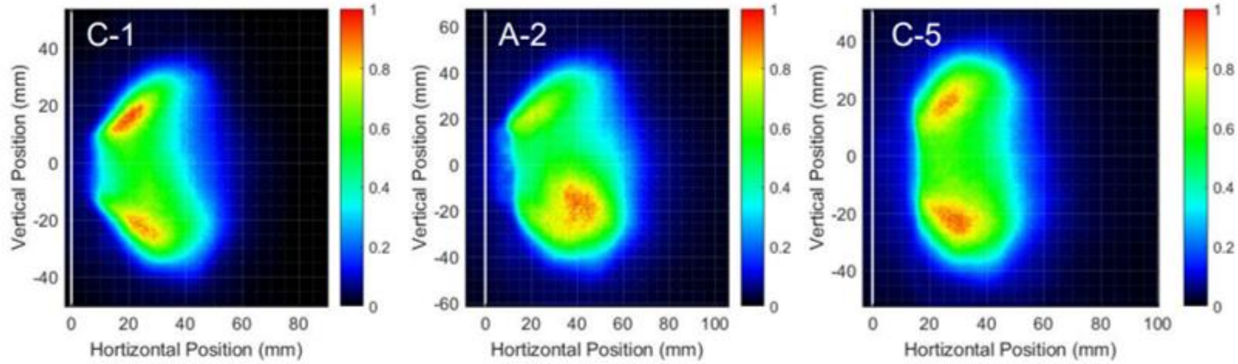


**Figure 4. Average normalized OH* image of C-1 (left), average normalized OH* image of A-2 (center), and average normalized OH* image of C-5 (right) [7]**

Clearly, it is important to develop an understanding of the sensitivity of the fuel distribution and flame structure on the fuel properties and the swirling turbulent flow prior to the deployment of a produced SAF in the aviation sector. Thus, it is critical to develop tools to assess the behavior of these fuels within realistic gas turbine combustors. High-fidelity Computational Fluid Dynamics (CFD) modeling is a powerful tool that can help investigate the interaction between the reacting flow, spray, and turbulence within gas turbines. These multi-scale interactions occur at a broad spectrum of length and time scales. A high-fidelity CFD model can resolve most relevant spatial and temporal scales and requires no additional models to couple the large and small-scale behaviors.

For many years, the prevailing numerical approach to resolving flow fields within gas turbine combustors was Reynolds-averaged Navier-Stokes (RANS) model where the governing equations are averaged or filtered, wherein fluctuations at all scales are dealt with by a turbulence model and could not be used to accurately capture the stable and off-normal behavior. With the advancement of high-fidelity numerical methods, large eddy simulations (LES) and direct numerical simulations (DNS) offer a more realistic representation of the internal turbulent flow compared to RANS. Indeed, LES has been employed by many researchers to investigate stable combustion, lean blow out and high altitude relight [6, 8-13]. Nonetheless, CFD simulations of gas turbine combustors are challenging. This is due to the requirement of modeling multiple physical phenomena (turbulence, spray, combustion) with complex internal geometries such as radial swirlers and atomizers. Additionally, the flow within such gas turbines is highly turbulent (Reynolds numbers ~ O (10,000)). For DNS, resolving the flow down to the Kolmogorov scale can lead to a large number of grid points (O ($10^8$-$10^9$)). In the case of wall-resolved LES, the number of grid points is lower. However, the computational time-step limitation is restrictive. The fast-moving swirling air flow leads to very small time scales, that make the LES simulations computationally expensive. Such resolutions necessitate the utilization of large-scale high performance computing infrastructures for investigating the fuel impacts within gas turbines. Almost all CFD work for gas turbines are performed using low-order codes and our literature review demonstrates a lack of high-fidelity wall resolved LES and DNS calculations. An INCITE award will enable us to advance the state-of-the-art in this scientific discipline. With Nek5000, a highly scalable code which accurately resolves complex geometries, the INCITE award will allow for a first-of-its-kind calculations of reacting flow in gas turbines to gain unprecedented insights on the governing physics of fuel distribution effects on flame and flow behavior.

The tasks proposed in the current proposal will contribute directly to the understanding of SAFs by utilizing LES of a realistic gas turbine combustor and DNS of a simplified swirl-stabilized burner.

## 1.2 Recent Achievements

To numerically simulate the effect of fuel properties on the combustion dynamics in gas turbine engines, there is a need for computational tools that have capabilities to model complex geometries with a high level of numerical accuracy and are able to leverage leadership computing resources. Nek5000, a leading high-order spectral element, open-source code [14] is well-suited to perform the tasks described in this proposal. In 2022, the PIs received a Director's Discretionary (DD) allocation on CRAY XC40 Theta system with a proposal titled "Development of high-fidelity simulations of gas turbine combustors for sustainable aviation applications". This allocation was used to develop a workflow to perform wall-resolved large eddy simulations (LES) of the flow in the ARC M1 combustor using Nek5000. This included developing high-fidelity meshes for resolving the flow, performing turbulent flow calculations to be validated using PIV measurements, and implementing capabilities to model the spray and combustion processes.

Body-fitted mesh with resolved boundary layers was constructed based on the Army Research Combustor-Midsize (ARC-M1) combustor geometry using CUBIT 15.5. The computational mesh for the ARC-M1 combustor is shown in Figure 5, with a total number of 1,133,464 spectral elements. A polynomial order of $N$ = 7 was used, which resulted in a total number of 580 million grid points. The maximum grid spacing was approximately 0.52 mm while the minimum was about 5.2 micron. The non-reacting flow of the ARC-M1 combustor was simulated based on the same conditions as the experiments by Wood et al. [15]. The main air flow rate is kept as 44.2 g/s whereas the dilution air flow rate is 11.1 g/s which is divided equally among the 8 dilution pipes. The air flows at all inlets are maintained at a temperature of 394 K. The Reynolds number of the main air inflow based on the inflow pipe diameter, $D$ = 42.3 mm, and mean inflow velocity, $U$ = 35.6 m/s, is approximately 58,200.

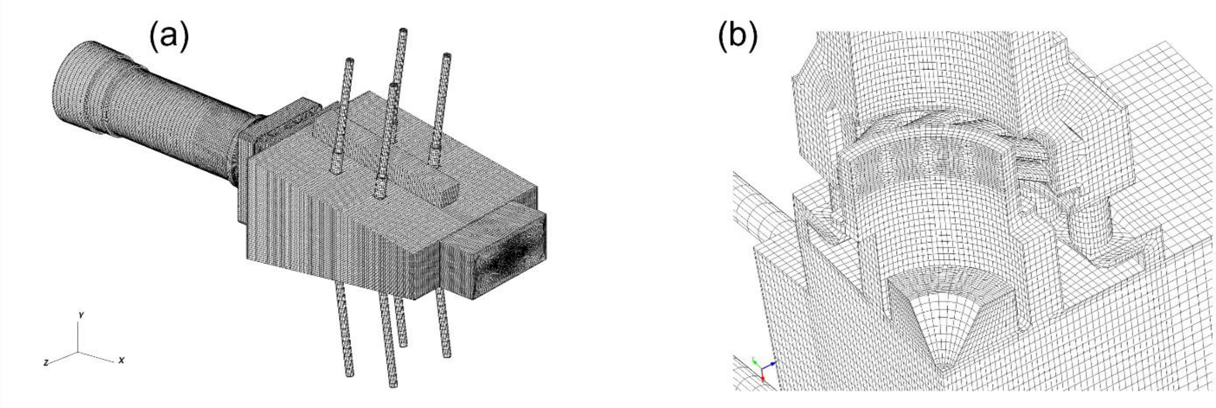


**Figure 5. Computational mesh for the ARC-M1 combustor. (a) Perspective view; and (b) zoomed view near the swirler.**

Wall-resolved LES of the flow in the ARC-M1 combustor was performed on 256 nodes (16,384 cores) of the Theta supercomputer. Figure 6 shows different views of the velocity magnitude in the ARC-M1 combustor at $t\ U/D$ = 10.4, which is about 16.1 flow-through time based on the combustor length and characteristic velocity scale in the combustor. By this time instant, the flow within the combustor has reached a statistically fully-developed state where complex interactions between the large- and small-scale turbulent structures are readily seen downstream of air flow entrances. In particular, high speed air flow is developed in the swirler core as shown in Figure 6a. This flow enters the combustor and expands radially outwards and meets the air stream that enters the combustor through the connector section. The interaction of the two air streams forms a small re-circulation zone in the vicinity of the combustor entrance as seen in Figure 6b and d. Another larger re-circulation region is created further downstream as the high velocity dilution air combines with the main flow leading to enhanced mixing within the combustor. Consequently, as shown by Figure 6c, larger shear rate is produced in this region that generates smaller-scale turbulent features compared to that at the center plane in Figure 6b.

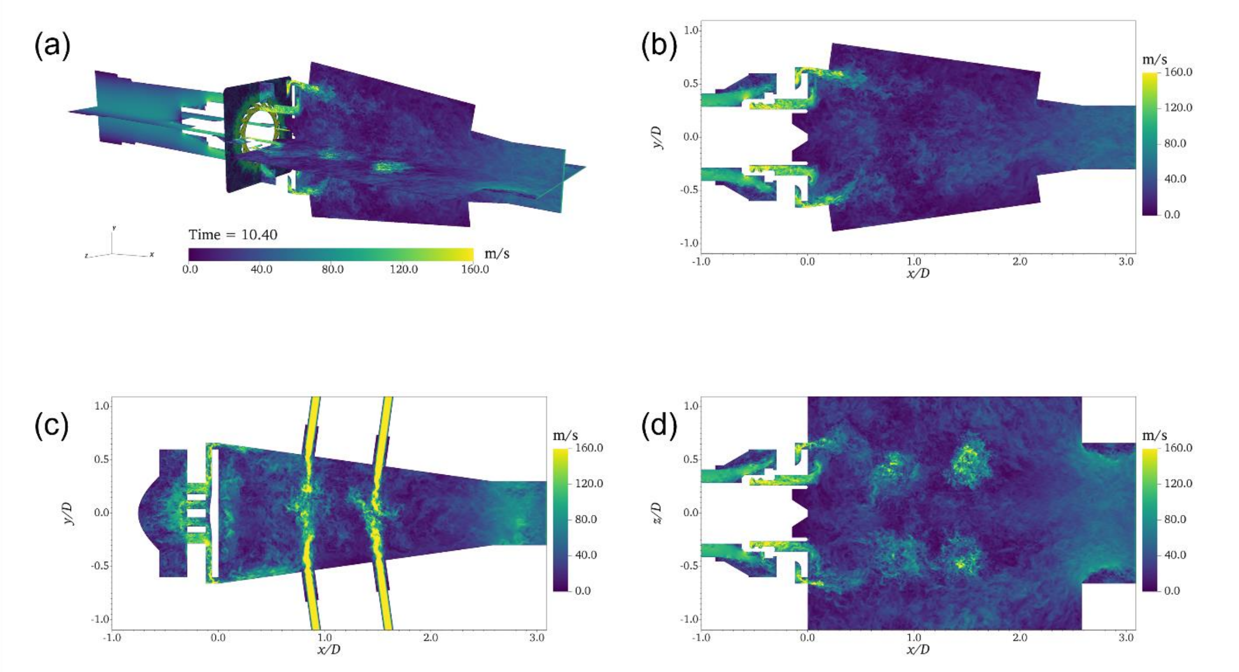


**Figure 6. Velocity magnitude in the ARC-M1 combustor at t U/D=10.4. (a) Perspective view; (b) z/D=0.0; (c) z/D=0.47 and (d) y/D=0.0**

The work done as part of the DD allocation clearly demonstrated the capability of Nek5000 to perform accurate scalable simulations of the highly turbulent flow inside gas turbine combustors. Validation of the simulations using PIV measurements is currently underway. Previous publications from the PIs have also shown accurate simulations of high-pressure sprays and combustion processes using Nek5000 [16-18]. We believe we have an accurate and scalable simulation tool as well as a demonstrated workflow ready to simulate the combustion dynamics in a gas turbine combustor. The simulation tasks proposed herein will be based on using this tool to investigate the challenges of using SAFs in gas turbine combustors.

## 2 RESEARCH OBJECTIVES AND MILESTONES

### 2.1 Objectives

The overall objective of this research is to develop a numerically accurate simulation framework to capture the flow and flame dynamics in a gas turbine combustor and the effect of fuel properties on these processes. Currently, no SAFs are available for large-scale end-use testing allowing for predictive modeling to play a critical role in assessing *apriori* behavior of newly produced fuels. In addition, the current state of simulations uses low-order methods for RANS and LES which limit the accuracy. The resources gained from this INCITE proposal will overcome these obstacles by generating high-fidelity data under gas turbine relevant operating conditions. The database will be generated through a hierarchy of direct numerical simulations (DNS) and wall-resolved large eddy simulations (LES) that can be used for scientific discovery, model development and validation. While the LES will provide critical insights on the overall change in flame shape, the DNS will provide unprecedented details of the flame structure that will enhance the understanding of conventional jet fuel v/s SAFs flames. Our objectives are motivated by seeking answers to the following overarching questions:

1. What are the effects of turbulence and flow structures on liquid and vaporized fuel distribution that would impact the flame stability?
2. How do the changes in properties between conventional jet fuel and SAFs impact the fuel distribution and the flame shape? What is the correlation between the fuel and the flame shape?
3. How is the flame structure of the partially premixed flame different for the two fuels? What fuel properties cause the observed changes?

### 2.2 Target Computational Problem: ARC-M1 Combustor and Swirl-Stabilized burner

The Army Research Combustor- Midsize (ARC-M1) was designed to replicate a single swirl-cup of a modern helicopter-sized gas turbine engine. Air is supplied to the ARC-M1 through two primary means: the main air, which flows through the dome from the air plenum, and the dilution air, which is split into four jets, two on each of the top and bottom of the combustor. The combustor is designed to operate similar to those in rich, quench, lean combustor designs [5]. For the combustor, the primary air flows in through a pipe of diameter 42.3 mm. The air flows downstream and splits into two regions: the swirler core and the connector section. The radial swirler with an approximate swirl number of 0.6 consists of air passages with elliptical holes with dimensions of 3.48 and 2.08 mm. The connector section consists of 28 cylindrical sections with 3.79 mm diameter. The air from the connector sections flows into the combustor through the annular cooling region. The dilution pipes have a diameter of 3.9 mm at the inflow and 5.4 mm closer to the combustor wall. The length of the combustor section is 109 mm. Closer to the inflow region, the combustor section is 55.6mm in width and 25.4mm near the outflow section. The geometry of the combustor is shown in Figure 7.

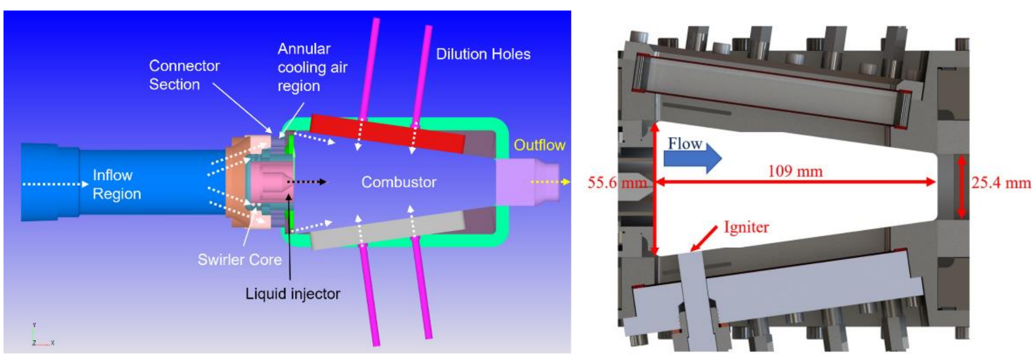


**Figure 7. Schematic of the computational domain with marked regions of the ARC-M1 (left) and, Schematic of the ARC-M1 with key dimensions highlighted (right) [15, 19]**

The ARC-M1 is designed with four-sided optical access, enabling a wide array of laser and optical diagnostics, which can be used to conduct high-speed flame imaging, air velocity measurements, and fuel spray characterization. The experimental data available for this combustor characterization of the non-reacting flow field using Particle Image Velocimetry, flame shape imaging using OH* chemiluminescence, spray droplet size and velocity distribution using X-ray diagnostics. Examples of these results are shown in Figure 8.

The proposed Direct Numerical Simulations (DNS) will be performed for a simplified swirl-stabilized burner that has all the typical flow features of typical gas turbine combustors. The generic swirl-stabilized spray burner with a pre-filming airblast atomizer was experimentally investigated by Grohmann et al. [20]. The schematic of the setup is shown in Figure 9. Air is supplied from a plenum to two swirlers that generate co-rotating flows in the inner and outer nozzle vanes. Fuel is sprayed onto the inner surface of the nozzle by a pressure-swirl atomizer which produces a hollow cone spray. The diameters of the inner and outer nozzle were 8 and 11.6 mm, respectively. The vertically standing combustion chamber had a cross section of 85 ×85 mm and a height of 169 mm. Experimental data for this setup includes Mie scattering, phase doppler interferometry (PDI) for spray characterization and chemiluminescence data for flame shape. Examples are shown in Figure 9.

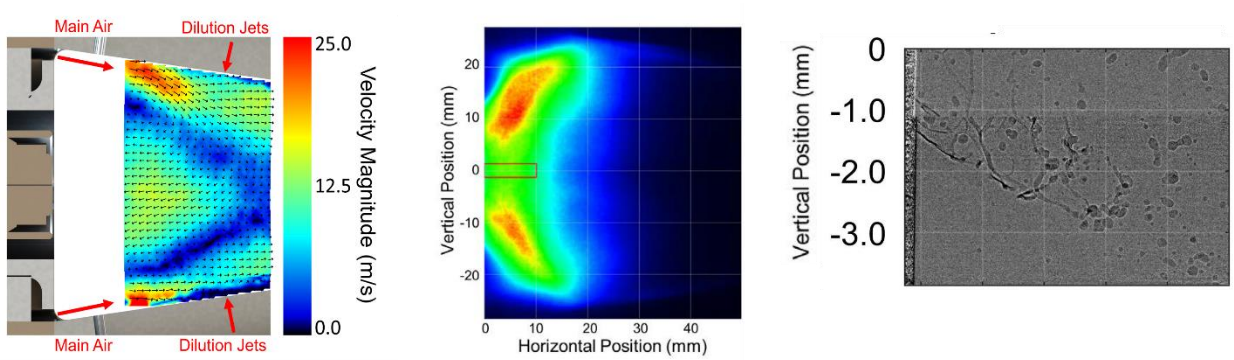


**Figure 8. Mean non-reacting flow field using PIV (left) Average OH* chemiluminescence (center) Near-nozzle X-ray spray imaging (right)**

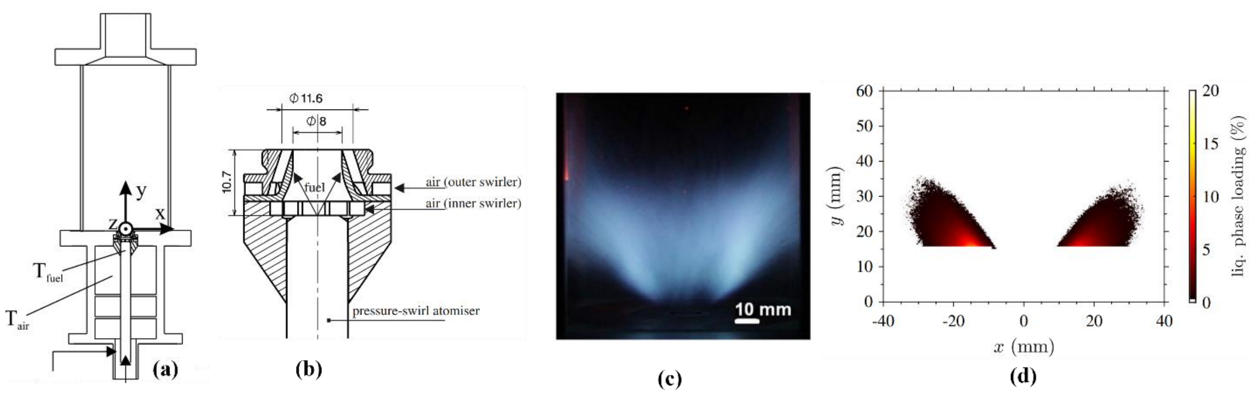


**Figure 9. (a) Schematic of the swirl-stabilized burner (b) Zoom in image of the atomizer and swirler (c) Line-of-sight integrated chemiluminescence image of flame (d) Liquid fuel distribution using PDI**

## 2.3 Computational Methods

### *2.3.1 Fluid Dynamics Solver: Nek5000*

In this proposal, we will employ Nek5000 to solve the low-Mach number compressible Navier-Stokes equations [21] coupled with thermal and species transport. These governing partial differential equations are discretized in space by using the spectral element method (SEM) [22], which combines the geometric flexibility of finite elements with the rapid convergence and tensor-product efficiencies of global spectral methods. Globally, the SEM is based on a decomposition of the domain into $E$ smaller subdomains (elements), which are assumed to be curvilinear hexahedra (bricks) that conform to complex domain boundaries found in the ARC-M1 combustor (Figure 7). Locally, functions within each element are expanded as $N^{th}$ order polynomials cast in tensor-product form, which allow differential operators on $N^3$ gridpoints per element to be evaluated with only $O(N^4)$ work and $O(N^3)$ storage.

The principal advantage of the SEM is that convergence is exponential in $N$, yielding minimal numerical dispersion and dissipation. This implies that significantly fewer grid-points per wavelength are required to accurately propagate a signal (or turbulent structure) over extended times associated with high Reynolds number simulations. The right image in Figure 9 shows a comparison between Nek5000 and another widely used open-source code in terms of accuracy and computational expense for a canonical flow problem [23]. It is shown that for a given accuracy, turbulent channel flow simulations performed with 7$^{th}$-order spectral elements require half as many gridpoints in each direction and were 10-times less expensive as compared to finite-volume-based simulations.

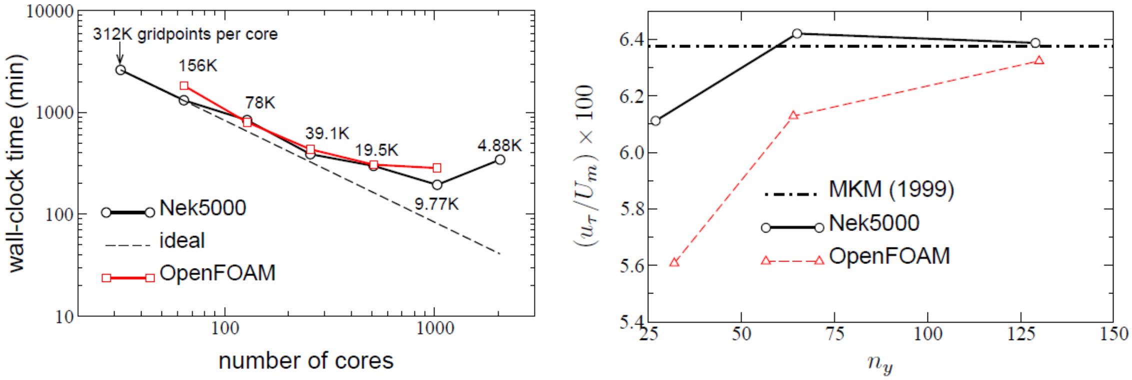


**Figure 10. Comparison of performance and accuracy of Nek5000 and OpenFOAM. These simulations were performed for a turbulent channel flow at a Reynolds number of 2800 [23] (left) Comparison of strong-scaling results on Intel Xeon 5570 cluster for the two codes. (right) Comparison of wall shear-stress for the two codes with increasing number of grids in the wall-normal direction ($n_y$). The dot-dashed line is the DNS result**

The simulation campaign will involve both wall-resolved LES and DNS calculations as noted below. For wall-resolved LES calculations, sub-models for fuel injection, spray, and combustion are necessary. The workflow to implement these model has already been established, as noted below. DNS will be performed for select conditions to provide “ground truth” data that will be subsequently used to improve combustion models. The low-Mach compressible formulation used by Nek5000 allows efficient characterization of flame and flow dynamics without being constrained by the low time steps required for resolving the acoustic timescales in fully-compressible formulations.

#### *2.3.2 Spray Solver*

In gas turbine combustors, the fuel is injected as a liquid spray through fuel injectors. These fuel sprays disintegrate into millions of droplets of size as small as 1 µm and then evaporates, mixes with air and undergo combustion. Numerical modeling of the spray needs to account for injection, breakup of the spray into ligaments and droplets, droplet collision and coalescence, and evaporation. As part of ALCC 2019, a parallel particle-in-cell library [24] was coupled with Nek5000 to model the spray droplets in a Lagrangian framework. The two-way coupling between the gas phase and liquid phase was achieved via spectral interpolation/projection procedures. The implementation has been validated for single-hole [17] and multi-hole [16] injectors under both non-vaporizing and vaporizing conditions. Figure 11 shows the validation of the spray model for a vaporizing multi-hole injection of the ECN Spray G under conditions relevant for internal combustion engines. It can be seen that the model performs very well under engine-relevant conditions. The spray setup has been recently ported to the ARC-M1 combustor setup and validation is currently underway.

#### *2.3.3 Combustion Solver*

Recent efforts have involved implementing capabilities into Nek5000 to model reacting flows. A Cantera-based chemical kinetics code was integrated into the Nek5000 simulation framework. This framework was used to perform DNS of a reacting jet in cross flow, which is a configuration relevant for gas turbine combustors. The simulations were shown [18] to predict the flow and combustion behavior accurately. Figure 12 compares the mean and RMS of the OH mass fraction, which is an indicator of the flame front, between the simulations and experiments. Both instantaneous and mean flame structures from the DNS agree with the experiment very well. The predicted two flame branches on the windward and leeward sides and their relative thicknesses also match the experimental observations. These results demonstrate good accuracy of the developed reacting flow solver in Nek5000.

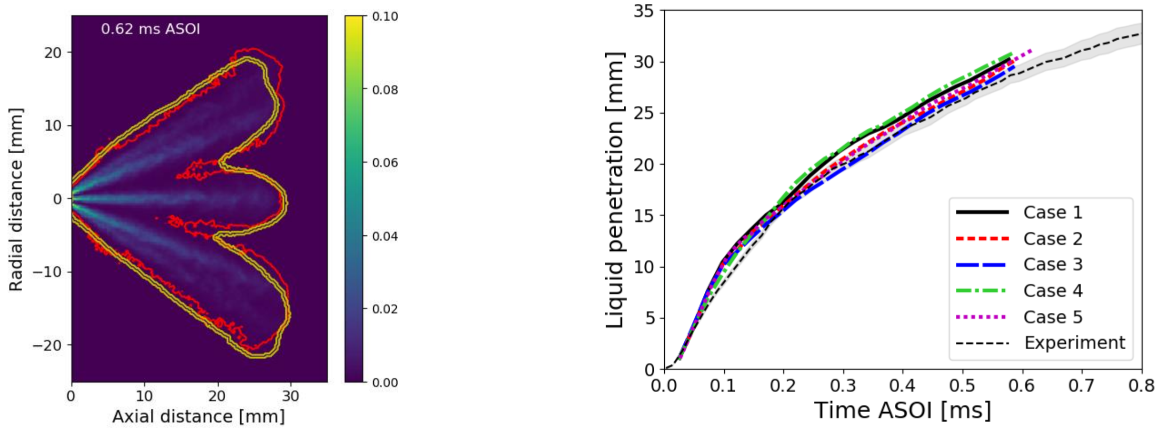


**Figure 11. Qualitative comparison of the jet structure observed from the shadowgraph experiment (top) and volume rendering of projected particle volume fraction from the Nek5000 simulation (bottom). (Right) Comparison of jet penetration between the simulation and experiment [16].**

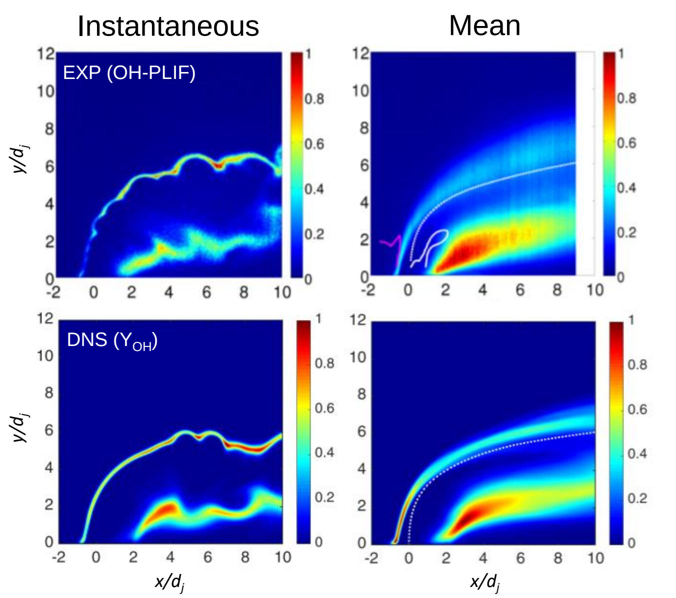


**Figure 12. Instantaneous and mean OH PLIF signals from the experiment (top) in comparison with instantaneous and mean OH mass fraction from the simulation (bottom). Experimental data is obtained from Wilde [25].**

## 2.4 Proposed Work

To meet our objectives, we will achieve three major milestones, which will be performed over the next one year. The project will heavily leverage the code improvements and capabilities achieved using the ALCC 2019 allocation. These milestones, described in the following paragraphs, are also summarized in the Milestone Table.

1. **Wall-resolved LES of ARC-M1 combustor using conventional jet fuel (A-2)**
**(20 flow through-times, 0.76M node-hours, 56 TB)**
LES will be performed using the compressible, low-Mach solver of Nek5000. The reacting simulation for this setup will leverage the non-reacting simulations highlighted under recent achievements. Experimentally measured spray droplet sizes and velocity distribution will be used for the spray model initialization. Detailed temperature-dependent thermo-physical properties (such as density, viscosity, heat of vaporization, surface tension, specific heat, vapor pressure, and thermal conductivity) will be used. The transport and liquid properties for Jet-A will be taken from literature [26]. To model the kinetics, a chemical mechanism for A-2 will be used [27]. The operating condition for this simulation will include liquid temperature of 300 K, fuel mass flow rate of 50 g/min, air temperature of 394 K, total air mass flow rate of 55.3 g/s and combustor pressure of 2 atm. The instantaneous and time-averaged liquid and vaporized fuel distribution, flame shape and flame anchoring location will be analyzed. In addition, the flame area and flame volume will be calculated by identifying the flame using edge-tracking approaches [28, 29]. Proper orthogonal decomposition will be performed to identify the dominant energy modes and structures for the non-reacting, non-reacting with spray, and reacting flow cases to understand how the introduction of spray and the heat release from the flame impact the turbulent structures in the combustor.
2. **Wall-resolved LES of ARC-M1 combustor using SAF surrogate**
**(20 flow through-times, 0.76M node-hours, 56 TB)**
The geometry and models noted in Task 1 will be used for performing LES of a SAF surrogate. One of the promising SAFs currently being produced is Hydroprocessed Ester Fatty acids- Synthetic Paraffinic Kerosene (HEFA-SPK). While the liquid properties of this SAF is available, chemical mechanisms and transport properties for HEFA-SPK are not available. Instead, n-butylcyclohexane (nBCH) will be chosen as the surrogate since its boiling range and auto-ignition characteristics are similar to HEFA-SPK [30]. Detailed temperature-dependent transport, liquid properties and chemical mechanism are available for this surrogate fuel [30]. Similar to Task 1, flame shape, flame area, flame volume, energy modes and structures analysis will be performed to shed light on how and why varying fuel properties lead to a change in the vaporization resulting in a change in flame shape.
3. **DNS of swirl-stabilized flame**
**(4 cases with 5 flow through-times, 0.94M node-hours, 54 TB)**
While changes in flame shape can be understood using LES, flame structure is not resolved. DNS of such flames can allow for ~20 grid points across the flame thickness resolving the flame structure. Liquid fuels lead to partially premixed flames and it is critical to ascertain the local flame structure to understand the flame's propensity to remain stable under challenging operating condition. The DNS will be performed for a simplified swirl-stabilized burner that has all the features in larger gas turbines such as an atomizer, co-rotating flows leading to the formation of multiple shear layers [10]. This configuration has been studied experimentally and spray droplet and velocity information are available [11]. The operating condition will include liquid temperature of 303 K, fuel mass flow rate of 14 g/min, air mass flow rate of 4.31 g/s and combustor pressure of 1 atm. Two air temperatures of 323K (above room temperature) and 268K (below room temperature) will be simulated. These two conditions will be simulated for two fuels i.e. A-2 and nBCH, thus totaling 4 DNS cases. Flame structure comparison using conditional means will be performed for both fuels to understand how and why varying fuel properties and air temperature changes the structure. This database of detailed flame structure can also be used for improving combustion models.

## 3. COMPUTATIONAL READINESS

The proposed production calculations outlined in section 2.4 include a description of the planned simulations and how they will help achieve the research objectives of this proposal. Node-hours and storage requirements for each milestone were also listed. This section gives detailed information on how these were determined.

### 3.1 Use of Resources Requested

In summary, the proposed simulation efforts fall into two categories: LES of the gas turbine combustor (Milestones 1 and 2) and DNS of swirl-stabilized flames to support sub-model development (Milestone 3). The total node-hour requirement will be **2.46 M Theta node hours** and the total storage requirement will be **166 TB**.

The equation below is used to arrive at the simulation cost for each Milestone and, therefore, each problem configuration.

$$\text{Theta Node-Hours per Milestone} = \alpha \times \beta \times \gamma \times \text{Total Flowthrough Time}$$

- The metric, $\alpha = \frac{\text{CPU}-\text{ms}}{\text{Gridpoints} \cdot \text{Timestep}}$ , represents a unit-cost per gridpoint per timestep for each simulation using Nek5000 and it is determined based on scaling studies performed on Theta which provide at least 70% parallel efficiency. More details on the scaling performance is described in Sec 3.3.

- The second metric, $\beta = \#\ \text{of Gridpoints}$, is based on using a polynomial order of N=7, which will be used for the production calculations.

- The third metric, $\gamma = \frac{\#\ \text{of Time}-\text{Steps}}{\text{Flowthrough time}}$, is the total number of time-steps per flowthrough time.

The storage requirements are based on single precision data (4 bytes) that is written to the standard Nek5000 field file and determined by the following equation:

$$\text{Storage per Milestone} = N_s \times 4 \frac{\text{Bytes}}{\text{Scalar}\cdot\text{Gridpoint}} \times \beta \times \text{Total Check-Point Files}$$

Where, $N_s$, are the total number of scalars which include the three components of velocity, pressure, temperature, and the species mass fractions. The chemistry mechanisms for jet fuel and SAFs will consist of approximately 30 species [27, 30]. Check-pointing will be performed 32 times per flow through time. Tables 1 and 2 summarizes the node-hour and storage requirements for each of the major milestones.

**Table 1. Summary table for resources requested. *For Milestone 3, the node-hours represents the cost of 4 DNS simulations as outlined in Sec 2.4**

| Milestone | CPU-ms Per Gridpoint Per Timestep | Avg. # of Gridpoints (M) | # of Time-Steps per Flowthrough time | # of Flowthrough times | CPU-Hours (M) | Node-Hours (M) |
|---|---|---|---|---|---|---|
| 1 | 7.05E-02 | 625 | 200,000 | 20 | 49 | **0.76** |
| 2 | 7.05E-02 | 625 | 200,000 | 20 | 49 | **0.76** |
| 3 | 7.05E-02 | 150 | 1,000,000 | 5 | 60 | **0.94*** |

**Table 2. Summary table for storage requested. *For Milestone 3, the storage represents the files generated from 4 DNS simulations as outlined in Sec 2.4**

| Milestone | # of Scalars | Avg. # of Gridpoints (M) | Checkpoint files per flowthrough time | # of Flowthrough times | Total Storage (TB) |
|---|---|---|---|---|---|
| 1 | 35 | 625 | 32 | 20 | **56** |
| 2 | 35 | 625 | 32 | 20 | **56** |
| 3 | 35 | 150 | 64 | 5 | **54*** |

## 3.2 Computational Approach

### *3.2.1 Fluid Dynamics Solver: Nek5000*

The "workhorse" solver for our proposed simulation campaigns will be the massively parallel code Nek5000 [14]. Nek5000 is a leading high-order spectral-element, open source code for accurate direct and large eddy simulations (DNS / LES) of fluid turbulence in complex domains with more than 400 registered worldwide users. It is a Gorden Bell Prize [31] winning code and was ranked first in 2010 and 2012 OECD/NEA thermal benchmark problems. Nek5000 has over a 100,000 lines of code and conforms to the FORTRAN (f77) and C ANSI standards and employs the MPI standard for parallelism. It is essentially a stand-alone code that has been ported and can run on numerous platforms from laptops to supercomputers. It is maintained in a Git repository and is automatically tested using four compilers and differing number of processors after each code update.

The solution procedure for solving the governing equations is based on a high-order splitting scheme [32], where the hydrodynamic equations are advanced with a backward difference/characteristic-based (BDF/CHAR), time-stepping algorithm. The BDF/CHAR scheme allows the simulation to overcome CFL restrictions imposed by standard schemes such as backward difference/extrapolation (BDF/EXT). Species and energy equations are integrated using CVODE from the SUNDIALS package. Nek5000 is also equipped with multilevel solvers that scale to millions of cores [33, 34]. The multilevel solvers require global coarse-grid solves that are based on either fast direct solvers developed in Tufo and Fischer [31] or the scalable algebraic multigrid formulation developed by Lottes [35]. The pressure sub-step requires a Poisson solve at each step, which is effected through multigrid-preconditioned GMRES iteration coupled with temporal projection to find an optimal initial guess. Particularly important components of Nek5000 are its scalable coarse-grid solvers that are central to parallel multigrid. Counts of 15-20 GMRES iterations per timestep for billion-gridpoint problems are typical with the current pressure solve.

Domain decomposition across all MPI ranks is central to enabling parallelism with Nek5000. In this case, the entire hexahedral mesh is partitioned at the element level and not finer. The data transfer amongst MPI ranks relies heavily on the open source GSLIB library [36]. GSLIB is a library for gather/scatter-type nearest neighbor data exchanges for SEM and FEM applications. For any global-to-local map, $l(i) = g(j(i))$, a matrix-vector product $l=\boldsymbol{Q}g$, where $Q$ is a Boolean matrix. GSLIB supports the parallel matrix-vector products, $Q$, $Q^T$, $QQ^T$. With the local-to-global mapping $j(i)$ on each MPI rank, GSLIB identifies shared global vertices across multiple processors and sets up the required communication exchange to use the fastest of three available algorithms. In addition, we will make use of GSLIB's scalable associative/commutative operators (+,*,min/max) for reduction, gather-scatter routines for arbitrary m-tuple (i.e. vector fields), and interpolation support for hexahedral spectral element meshes.

I/O is integrated efficiently into Nek5000. Nek5000 makes use of application-level check-pointing and has a built-in, self-contained, parallel I/O capability for restart and output of case specific data analysis. For the simulations proposed in this project, checkpointing is accomplished by writing the standard Nek5000 field-file (a.k.a check-point file) at time-steps corresponding to 1/32 of the flowthrough time which represents <0.1% of the time-steps in a given engine simulation. As a result, Nek5000 is not I/O bound where I/O time is negligible compared to the total simulation time. Nek5000 implements two I/O strategies: one based on MPI-I/O and another with no dependencies that collects reads and writes on a subset of the MPI ranks to reduce congestion. Check-point files are saved in single-precision format to save the disk space with 20 - 40 bytes required per grid-point. Nek5000 solves the governing equations in dimensionless and normalized form, the error induced by single precision output is typically negligible at the post-processing stage.

Visualization is performed on the *Cooley* cluster at ALCF. This project will make use of the full-suite of visualization software to accelerate scientific discovery inside gas turbines. In collaboration with the visualization team at the ALCF, we will use the VisIt parallel tool to extract qualitative flow-field information and improve our understanding of the flow physics during the unsteady combustion processes. This type of analysis scales well on Cooley and we expect to use 40 - 80 nodes to meet our post-hoc visualization needs.

#### ***3.2.2*** *Next-generation fluid flow solver: nekRS*

As the upcoming exascale machines at the DOE leadership computing facilities are all heterogeneous, accelerator-based architectures, the fluid flow solvers also need to be scalable on this new hardware. As part of the developmental work for future INCITE proposals, nekRS will be used to perform preliminary simulations on the upcoming ALCF Polaris platform. nekRS is an open-source Navier Stokes solver based on the spectral element method targeting modern processors and accelerators, and is being developed under the DOE ECP program. The code uses the CEED [37] software products OCCA and libParanumal. The Open Concurrent Compute Abstraction (OCCA) [38] layer in nekRS, is an open-source library that makes it easy to program different types of devices (e.g. CPU, GPU, FPGA). It provides a unified API for interacting with backend programming models (e.g. CUDA, OpenMP, OpenCL, HIP). OCCA also offers runtime compilation of compute kernels with just-in-time (JIT) optimization, which is particularly important for high-order methods where inner-most loops have bounds depending on the order.

nekRS currently has most of the capabilities of Nek5000 including the solution of incompressible and low-Mach-number Navier Stokes with thermal and scalar transport. nekRS also supports several LES and RANS turbulence models and supports data analysis and visualization through VisIt and Paraview. It supports MPI+X hybrid parallelism using CPU, CUDA, HIP and OPENCL. The code is still under early prototype and some of the important features necessary for gas turbine engine simulations such as the Lagrangian capability for spray modeling are still under development. Developmental activities external to this INCITE proposal over the next year will ensure that the code will be ready for production simulations in the next year on Aurora. This is discussed further in the "Developmental Work" subsection (Sec 3.4).

### 3.3 Parallel Performance

The entire computational infrastructure of Nek5000 is supported with the MPI model for parallelism. Extensive benchmark analysis of Nekbone, a conjugate gradient (CG) solver and a light-weight version of Nek5000, was performed for the Cray XC40 machine *Theta* [39]. Strong scaling analysis on simple geometries (i.e. boxes), for local node-level workloads comparable to our gas turbine simulations, indicated that no substantial reduction in time-to-solution was gained with the hybrid MPI + OpenMP model. As a result, we have found the best results with using 64 MPI-only tasks per Knight's Landing (KNL) node with one rank per core. We also make use of the support for 512-bit Advanced Vector Extensions (AVX-512) where we have seen an approximate 2 times performance boost over AVX for similar mathematical operations. Based upon our ALCC 2019 and INCITE 2021 allocations we have typically used "cache" memory mode for KNL. The PIs have maintained strong collaboration with the ALCF Catalyst team over the past few years. This has led to continuous integration and development to create frameworks within Nek5000 to tackle complex applications such as internal combustion and gas turbine engines.

Figure 12a shows the inter-node, strong-scaling performance of Nek5000 for non-reacting simulations of the ARC-M1 combustor for different polynomial orders. The mesh setup, as described in Sec 1.2, consists of E=1,133,464 spectral elements. This corresponds to 240M, 570M, and 1.11B grid points for polynomial orders, $N$=5, $N$=7, and $N$=9 respectively. The problem ran for 200 timesteps starting from a fully developed flow configuration. The y-axis shows the average wall-time per timestep. It is seen that the problem is able to scale well on up to 512 nodes with more than 80% efficiency for $N$=9. Figure 12b shows the strong scaling performance of reacting simulations within the ARC-M1 combustor. The simulation setup is similar to the setup used for the scaling study in Figure 13 but includes 4 species and a single-step chemistry. It is seen that the inclusion of chemical kinetics did not affect the strong scaling performance of the simulations. The addition of chemistry led to a 10% increase in computational cost. As part of ALCC 2019, the strong-scaling performance of the chemical kinetics solvers within Nek5000 have been verified to scale well on mechanisms with >50 species. For the production LES and DNS simulations described in Sec 2.4, the chemistry mechanism is expected to consist of ~30 species and ~200 reactions. The node hour estimates in Sec. 2.4 were estimated based on the assumption that with the inclusion of this chemistry mechanism, the simulations will become ~7x more expensive (due to 1.4x increase in time per timestep and 5x reduction in timestep).

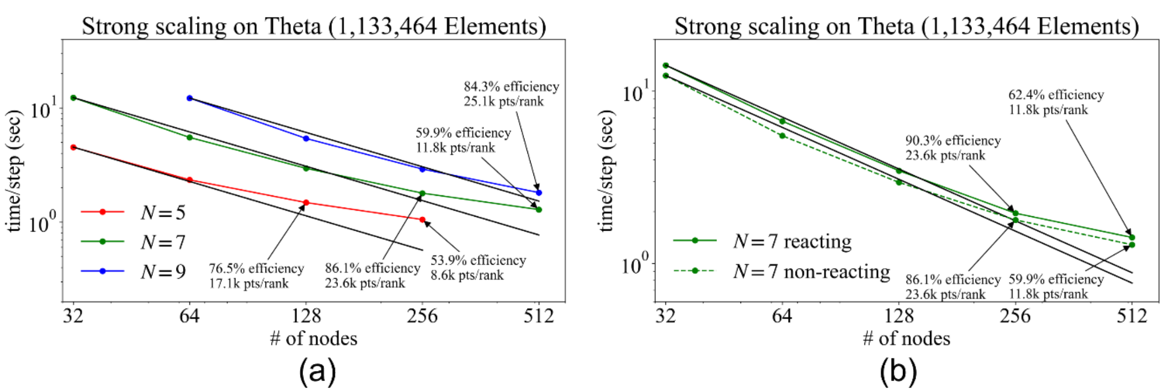


**Figure 13. Inter-node strong-scaling plots of Nek5000 on Theta for the ARC-M1 combustor for (a) non-reacting and (b) reacting conditions.**

## 3.4 Developmental Work

### *3.4.1 Porting spray and chemistry models to nekRS*

As part of the efforts to port the simulations to the next-generation computing architectures, spray and chemistry submodels will be integrated into the nekRS code. This will be enabled through the OCCA unified API where device abstractions are created to reflect the physical model evaluations in the nested-loop structure associated with high-order, spectral elements. For the Lagrangian spray sub-models, we will make use of the developments within the ECP CoPA Cabana framework [40]. For the implementation of chemistry mechanisms that are scalable on GPUs, the Zero-RK solvers [41] will be utilized. These developments will occur on ALCF Polaris machine using a DD allocation. This work will be carried out in collaboration with Saumil Patel from Argonne National Laboratory.

### *3.4.2 Virtual and Augmented Reality Framework for Gas Turbine Simulations*

The visualization team at Argonne National Laboratory is developing virtual and augmented reality simulation frameworks that can assist modelers in gaining invaluable insights into the simulations in real-time. For the gas turbine simulations planned in this proposal, having full 3D access to the simulation dataset through virtual/augmented reality can help the simulation in a few different ways: (i) identify regions of the simulation domain which are under-resolved and needs to be remeshed with increased resolution, (ii) identify, in real-time, the effect of spray injection rates and upstream geometry features on the flow and flow-spray interactions, and (iii) develop an improved understanding of the lean blow-out process, which includes a complex interplay between spray cooling, chemical kinetics, and turbulence. As part of the developmental work, Nek5000 will be instrumented with this framework and will be used to gain new insights into the unsteady combustion processes.

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## PERSONNEL JUSTIFICATION AND MANAGEMENT PLAN

### PERSONNEL JUSTIFICATION

The project team consists of Dr. Muhsin Ameen (PI), Dr. Debolina Dasgupta (co-PI) and Dr. Sicong Wu (co-PI). Dr. Ameen is the lead PI and will be responsible for the overall project management. He has over 10 years of experience in high performance computing, high-fidelity simulations, and turbulent combustion modeling. He has significant expertise in using Nek5000 for performing high-fidelity device-level simulations on leadership-class supercomputers. He has previously served as the PI on an ALCC 2019 allocation, a co-PI on an INCITE 2021 allocation and PI on multiple DD allocations. Dr. Dasgupta is a co-PI and will be responsible for the data analysis for the simulations performed. She has extensive background in large-scale data analysis facilitating understanding and model development for turbulent-chemistry interactions and combustion dynamics. Her recent efforts include device-level modeling of gas turbines for aviation and stationary power generation. Dr. Wu is a co-PI and will lead the technical development of Nek5000, perform high-fidelity simulations. He has research background in turbulence modeling and high-performance computing. He has extensive experience in high-fidelity simulations using Nek5000, turbulence wall modeling and large-scale data analysis. His recent efforts include advancing the capabilities of Nek5000 for modeling complex multi-physics processes in gas turbines, heat transfer in impinging jet and spray-flow interactions.

The project will also leverage several strong collaborations that the PIs have built over the years. Dr. Saumil Patel from ANL will be providing guidance on implementing schemes to speed up the simulations on the ALCF architecture. The gas turbine team from UIUC led by Prof. Tonghun Lee will be consulted for providing the combustion experimental data used for validating the reacting flow simulations. Chris Powell from Argonne will provide X-ray experimental measurements for validating the spray models. Dr. Paul Fischer from UIUC (chief architect of Nek5000 and NekRS) will be involved in providing guidance in the project progress and implementing new capabilities that can speed up the simulations. Mr. Insley and Dr. Rizzi from ANL are also collaborators to this project and will provide expertise in in-situ analysis and visualization tasks. Guidance for NekRS development and performance on Aurora will be provided through interactions with the performance engineering team at ALCF. The project is tightly aligned with the SAF efforts funded by DOE VTO and thus involves collaboration with multiple experimentalists and other modelers who will be leveraging the datasets generated for developing lower order models.

### MANAGEMENT PLAN

Dr. Ameen will be responsible for the overall project management, completion of the project milestones, and ensuring that the node-hour and storage usage are proceeding as planned. He will be coordinating with Dr. Dasgupta to ensure that the simulation results feed into the research activities being performed within VTO’s SAF program. Dr. Wu, with help from the ALCF catalyst team, will ensure that the solver settings, preconditioners, etc. are chosen optimally to ensure fastest time-to-solution. Dr. Ameen, with support from members within the TAPS division, will be responsible for coordinating the integration of suitable fuel chemistry mechanisms to the simulation framework. Dr. Dasgupta will be coordinating with the gas turbine and X-ray experimental teams to provide sufficient validation datasets for the simulations. The entire team will be working with the ALCF catalyst team to extend the modeling framework to the next-generation Polaris and Aurora architectures.

**Proposal Title (exactly as it appears on submission):** DNS and LES of Gas Turbine Combustors for Sustainable Aviation Fuels

| **Year 1** | | **Total number of node-hours for Year 1:** *2.46 M* | |
|---|---|---|---|
| **Milestone:** | **Details (as appropriate):** | **Dates:** | **Status: (renewals only)** |
| **1. Wall-resolved LES of ARC-M1 combustor using conventional jet fuel (A-2)** | **Resource:** Theta **Node-hours:** 0.76 M<br>**Production size runs (number of nodes):** 256<br>**Filesystem storage (TB and dates):** 56 TB, 1/23 – 12/23<br>**Archival storage (TB and dates):** 60 TB, 1/23 – 6/24<br>**Software Application:** Nek5000<br>**Tasks:** (i) Perform production simulations of 20 flowthrough times; (ii) Archive check-point data; (iii) Analysis of results using visualization software (e.g. VisIT, ParaView, etc) and POD; (iv) Archive analysis check-point data<br>**Dependencies:** None | *1/23 – 6/23* | |
| **1. Wall-resolved LES of ARC-M1 combustor using SAF surrogate** | **Resource:** Theta **Node-hours:** 0.76 M<br>**Production size runs (number of nodes):** 256<br>**Filesystem storage (TB and dates):** 56 TB, 7/23 – 12/23<br>**Archival storage (TB and dates):** 60 TB, 7/23 – 6/24<br>**Software Application:** Nek5000<br>**Tasks:** (i) Perform production simulations of 20 flowthrough times; (ii) Archive check-point data; (iii) Analysis of results using visualization software (e.g. VisIT, ParaView, etc) and POD; (iv) Archive analysis check-point data<br>**Dependencies:** Completion of Milestone 1 | 7/23 – 12/23 | |
| **3. DNS of swirl-stabilized flame** | **Resource:** Theta **Node-hours:** 0.94 M<br>**Production size runs (number of nodes):** 512<br>**Filesystem storage (TB and dates):** 54 TB, 3/23 – 12/23<br>**Archival storage (TB and dates):** 60 TB, 3/23 – 6/24<br>**Software Application:** Nek5000<br>**Tasks:** (i) Perform production simulations of 4 DNS cases; (ii) Archive check-point data; (iii) Analysis of results using visualization software (e.g. VisIT, ParaView, etc) and POD; (iv) Archive analysis check-point data<br>**Dependencies:** None | 3/23 – 9/23 | |

## PUBLICATIONS RESULTING FROM INCITE AWARDS

1. S. Wu, M.M. Ameen, S.S. Patel, ‘Investigating the origins of Cyclic Variability in Internal Combustion Engines using Wall-resolved Large Eddy Simulations’, *ASME Internal Combustion Engine Fall Conference*, October 2021, ICEF2021-67671
2. S. Wu, M.M. Ameen, S.S. Patel, ‘Investigation of cycle-to-cycle variations in internal combustion engine using proper orthogonal decomposition’, *Flow, Turbulence and Combustion* (under review), 2022.
3. M.M. Ameen, S. Patel, J.D. Colmenares, and S. Wu, ‘Direct Numerical Simulation (DNS) and High-Fidelity Large-Eddy Simulation (LES) for Improved Prediction of In-Cylinder Flow and Combustion Processes,’ *2021 DOE VTO Annual Merit Review*, June 2021.

**Curriculum Vitae**
**Muhsin Ameen**
**mameen@anl.gov**

## PROFESSIONAL PREPARATION

PhD in Mechanical Engineering Dec 2014
*Purdue University, West Lafayette, IN*

ME in Mechanical Engineering May 2010
*Indian Institute of Science, Bangalore, Karnataka, India*

BTech in Mechanical Engineering Apr 2008
*National Institute of Technology, Calicut, Kerala, India*

## APPOINTMENTS

*Argonne National Laboratory (February 2015 – Present)*
- Senior Research Scientist *(April 2020 - Present)*
- Research Scientist *(October 2019 – April 2020)*
- Mechanical Engineer *(August 2017 – September 2019)*
- Postdoctoral appointee *(February 2015 – July 2017)*

*Purdue University (September 2010 – December 2014)*
- Graduate Research Assistant

## FIVE PUBLICATIONS MOST RELEVANT TO THIS PROPOSAL

4. A.C. Nunno, S. Wu, **M.M. Ameen**, P. Pal, P. Kundu, A. Abouhussein, Y. Peet, M. Joly, and P. Cocks. "Wall-Resolved LES Study of Shaped-Hole Film Cooling Flow for Varying Hole Orientation." In *AIAA Scitech 2022* Forum, p. 1404. 2022.
5. J.D. Colmenares, **M.M. Ameen**, and S.S. Patel, 'Large Eddy Simulation of Gasoline Sprays in a Lagrangian-Eulerian Framework Using the High-order Spectral Element Method', *ASME Internal Combustion Engine Fall Conference*, October 2021, ICEF2021-67848.
6. J.D. Colmenares, **M.M. Ameen,** and S. S. Patel. "Large-eddy simulation of non-vaporizing sprays using the spectral-element method." *International Journal of Multiphase Flow* (2022): 104155.
7. C. Xu, **M.M. Ameen**, P. Pal, and S. Som, "Direct Numerical Simulation of a Reacting Hydrogen Jet in Turbulent Vitiated Crossflow Using Spectral Element Method." In *AIAA SCITECH 2022 Forum* (p. 0823).
8. S. Wu, **M.M. Ameen**, S.S. Patel, 'Investigating the origins of Cyclic Variability in Internal Combustion Engines using Wall-resolved Large Eddy Simulations', *ASME Internal Combustion Engine Fall Conference*, October 2021, ICEF2021-67671

## RESEARCH INTERESTS AND EXPERTISE

**Dr. Muhsin M. Ameen** is a senior research scientist in the Center for Advanced Propulsion and Power in Argonne's TAPS division, where his work focuses on developing techniques to improve the accuracy and turnaround time of computational fluid dynamics (CFD) simulations of automotive and gas turbine engines. He served as the PI on the DOE Vehicle Technology Office (VTO) funded task titled "Developing a framework for performing high-fidelity engine simulations using Nek5000 code". He was also the PI for an ALCC 2019 and a co-PI for the INCITE 2021 allocations which granted more than 150 Million core hours on ALCF Theta to perform the simulations for this VTO task. His research interests include developing high-order computational codes for CFD, high performance computing, combustion modeling and machine learning. At Argonne, Dr. Ameen has been a recipient of several awards including the 2018 FLC Technology Transfer award, the 2017 postdoctoral performance award and the 2016 Pacesetter award. Dr. Ameen received his PhD from Purdue University (2014) in Mechanical Engineering, with specialization in computational fluid dynamics applications for engines with a specific focus on turbulence chemistry interaction modeling and high-performance computing. He joined Argonne as a postdoctoral fellow in 2015, and was subsequently converted to staff in 2017.

## SYNERGISTIC ACTIVITIES

1. Co-lead for the Combustion/Kinetics team for the PACE consortium: responsible for coordinating the research efforts in combustion/kinetics across 5 national laboratories
2. Session chair/co-chair for SAE, ASME and Combustion Institute conferences
3. Reviewer for Journals: Combustion and Flame, Combustion Science and Technology, Combustion Theory and Modeling, Physics of Fluids, Fuel, SAE International Journal of Fuels and Lubricants, Computers and Fluids, Applied Mathematical Modeling
4. Reviewer for DOE Funding Proposals: VTO SBIR, ALCC
5. Thesis committee member for two PhD students

## COLLABORATORS (*PAST 5 YEARS INCLUDING NAME AND CURRENT INSTITUTION*)

Som, Sibendu; Patel, Saumil; Pal, Pinaki; Xu, Chao; Scarcelli, Riccardo; Powell, Chris; Kim, Joohan; Dasgupta, Debolina (Argonne National Laboratory)
Zhang, Yu; Zhang, Anqi; Pei, Yuanjiang; Zhao, Emma (Aramco Services Company)
Yazdani, Miad; Cocks, Peter (Raytheon Technologies Research Center)
Senecal, Peter; Pomraning, Eric; Probst, Daniel; Wijeyakulasuriya, Sameera (Convergent Science, Inc.)
Ihme, Matthias (Stanford University)
Whitesides, Russell; McNenly, Matthew (Lawrence Livermore National Laboratory)
Lu, Tianfeng (University of Connecticut)
Moiz, Ahmed (DataRobot)
Lavertu, Thomas; Klingbeil, Adam (Wabtec)
Pickett, Lyle; Charles Mueller, Sjoberg, Magnus; Jackie Chen (Sandia National Laboratories)
Millo, Federico (Politecnido di Torino)
VanderWege, Brad; Ting, Foochern; Iyer, Claudia (Ford),
Wei, Haiqiao (Tianjin)
Wang, Zhiyan (ExxonMobil)
Abraham, John (SDSU)
Owoyele, Ope (LSU)
Kundu, Prithwish (Euler Motors)
Yang, Xiaofeng; Grover, Ron (GM)
Kodavasal, Janardhan (Cummins)
Colmenares, Juan (General Atomics)

**DEBOLINA DASGUPTA**
**Transportation and Power Systems Division**
**Argonne National Laboratory**
**9700 S. Cass Ave, Lemont, IL 60439**
ddasgupta@anl.gov; (630) 252-3033

## PROFESSIONAL PREPARATION

Ph.D., Aerospace Engineering, Georgia Institute of Technology, September 2018
MS, Aerospace Engineering, Indian Institute of Technology Madras, India July 2014
BE, Mechanical Engineering, Jadavpur University, India, June 2011

## APPOINTMENTS

*Argonne National Laboratory (November 2018 – Present)*

- Research Scientist *(November 2021 – Present)*
- Postdoctoral appointee (*November 2018 – October 2021)*

*Georgia Institute of Technology (August 2014 – September 2018)*

- Graduate Research Assistant

## FIVE PUBLICATIONS MOST RELEVANT TO THIS PROPOSAL

6. **Dasgupta, D.,** Som, S., Wood, E., Lee, T., Mayhew, E., Temme, J., Kweon, C-B., "Computational Fluid Dynamics Modeling of Fuel Properties Impact on Lean Blowout in the ARC-M1 Combustor", Proceedings of ASME Turbo Expo 2022, Paper No. GT2022-79347
7. **Dasgupta, D.,** Som, S., Wood, E., Lee, T., Mayhew, E., Temme, J., Kweon, C-B., "Computational Fluid Dynamics Modeling of Lean Blowout Dependence on Operating Conditions in the ARC-M1 Gas Turbine Combustor", 2022 Spring Technical Meeting of the Central States Section of the Combustion Institute.
8. **Dasgupta, D.,** Som, S. Wood, E. Lee, T., Mayhew, E., Temme, J. Kweon, C-B., "X-ray Data Enabled Improved Near Nozzle Spray Validation for ARC-M1 Combustor" 2022 AIAA Science and Technology Forum and Exposition, January 3-7 2022, San Diego, California
9. **Dasgupta, D.,** Sun, W., Day, M., Aspden, A., Lieuwen, T. "Analysis of chemical pathways and flame structure for n-dodecane/air turbulent premixed flames", *Combustion and Flame* 2019, 207, 36-50.
10. Amato A., Day M., Cheng R.K., Bell J., **Dasgupta D.**, Lieuwen T., "Topology and burning rates of turbulent lean $H_2$/Air flames", *Combustion and Flame* 2015, 162(12) 4553-4565.

## RESEARCH INTERESTS AND EXPERTISE

**Dr. Debolina Dasgupta** is a Research Scientist in the Center for Advanced Propulsion and Power in Argonne National Laboratory's Transportation and Power Systems Division. Her expertise includes Direct Numerical Simulations, and device level Computational Fluid Dynamics modeling, High Performance Computing, and large-data analysis facilitating understanding and model development for turbulent-chemistry interactions, combustion dynamics, thermo-acoustic instability in gas turbine engines for aviation and stationary power generation applications. She serves as a co-PI on DOE Vehicle Technology Office funded task on "Sustainable Aviation Fuels". At Argonne, Dr. Dasgupta has received the Argonne Impact Award for Program Development in 2022

## SYNERGISTIC ACTIVITIES

1. American Society of Mechanical Engineers (ASME)- International Gas Turbine Institute's Combustion, Fuels and Emissions Committee Member (June 2022 – Present)
2. Served as Colloquium Co-Chair for Propulsion for 39th Combustion Symposium
3. Invitee to National Academy of Engineering (NAE) 2022 US Frontiers of Engineering Symposium (only 100 people between ages 30-45 are invited) to be held in September 2022
4. Panelist in the Combustion, Heat Transfer, and Emissions panel in the Sustainable Aviation Fuel end-use Workshop held at Argonne National Laboratory in February 2022.
5. Member of American Institute of Aeronautics and Astronautics (AIAA), Combustion Institute
6. Served as Session chair for ASME Turbo Expo since 2019, Session chair for Combustion Institute Conferences since 2019
7. Organized Women in Combustion networking event at the 12th U.S. National Meeting of the Combustion Institute
8. Reviewer for Combustion and Flame, Fuels, Energy and Fuels, ASME Journal for Gas Turbines and Power, Proceedings of the Combustion Institute, ASME Turbo Expo

## COLLABORATORS (*PAST 5 YEARS INCLUDING NAME AND CURRENT INSTITUTION*)

Som, Sibendu; Pal, Pinaki; Torelli, Roberto; Powell, Chris; Longman, Doug; Ameen, Muhsin; Sforzo, Brandon; Nocivelli, Lorenzo, Paulson, Noah; Lusch, Bethany; Zhang, Yuepeng; Blaizik, Ben; Schwarting, Marcus; Foster, Ian; Biruduganti, Munidhar; Supekar, Sarang (Argonne National Laboratory)
Senecal, Peter; Pomraning, Eric; Probst, Daniel; Drennan, Scott; Kumar, Gaurav; Wijeyakulasuriya, Sameera; Coil, Millicent; Convergent Science, Inc.)
Lieuwen, Timothy; Sun, Wenting (Georgia Institute of Technology)
Day, Marc (National Renewable Energy Laboratory)
Venkastesan, Krishna; McManus, Keith; Kim, Kwanwoo (General Electric)
Klinzing, William; Flage, Alex (3M)
Mayhew, Eric; Temme, Jacob; Kweon, Chol-Bum (Army Research Laboratory)
Lee, Tonghun (UIUC)
Agrawal, Ajay (University of Alabama)
Aspden, Andrew (Newcastle University)
Stelmakh, Veronica; Chan, Walker (Mesodyne Inc.)

**Curriculum Vitae**

**Sicong Wu**
**Transportation and Power Systems Division**
**Argonne National Laboratory**
**9700 S Cass Ave, Lemont, IL 60439**
**wus@anl.gov**

## PROFESSIONAL PREPARATION

Ph.D., University of Illinois at Urbana-Champaign, Theoretical and Applied Mechanics, May 2020
M.S., University of Illinois at Urbana-Champaign, Theoretical and Applied Mechanics, May 2016
B.S., University of Minnesota at Twin-Cities, Mechanical Engineering, May 2013

## APPOINTMENTS

| | | |
|---|---|---|
| May 2020–present | Postdoctoral Appointee | Argonne National Laboratory |
| Jan 2014–May 2020 | Graduate Research Assistant | University of Illinois at Urbana-Champaign |

## FIVE PUBLICATIONS MOST RELEVANT TO THIS PROPOSAL

1. A.C. Nunno, **S. Wu**, M. Ameen, P. Pal, P. Kundu, A. Abouhussein, Y. Peet, M. Joly, and P. Cocks. "Wall-Resolved LES Study of Shaped-Hole Film Cooling Flow for Varying Hole Orientation." In *AIAA Scitech 2022* Forum, p. 1404. 2022.
2. **S. Wu**, S. S. Patel, M. M. Ameen, 'Investigating the origins of Cyclic Variability in Internal Combustion Engines using Wall-resolved Large Eddy Simulations', *ASME Internal Combustion Engine Fall Conference*, October 2021, ICEF2021-67671.
3. M. M. Ameen, **S. Wu**, and S. Patel, 'Development and Validation of Nek5000 for High-Fidelity Engine Simulations,' *Virtual AEC Program Review Meeting*, February 2021.
4. J. D. Colmenares, M. M. Ameen, **S. Wu**, and S. Patel. "Large Eddy Simulation of Turbulent Particle-laden Jets using the Spectral Element Method." In *AIAA Scitech 2021* Forum, p. 0635. 2021.
5. S. Patel, M. Ameen, T. Chatterjee, and **S. Wu**. "Large Eddy Simulations of Internal Combustion Engines to Understand the Origins of CCV." Bulletin of the American Physical Society 65 (2020).

## RESEARCH INTERESTS AND EXPERTISE

Dr. Sicong Wu is a Postdoctoral Appointee in the TAPS division, with research background in turbulence modeling and high-performance computing. He has extensive experience in direct numerical simulation using Nek5000, turbulence wall modeling and large-scale data analysis. Recent research efforts include advancing the capabilities of Nek5000 for the internal combustion engines and gas turbine combustors on DOE leadership supercomputer platforms, modeling heat transfer in impinging jet flow and spray-flow interactions.

## SYNERGISTIC ACTIVITIES

1. Member of American Physical Society (APS), American Society of Mechanical Engineers (ASME)
2. Principal Investigator (PI) of the Laboratory Directed Research and Development (LDRD) Project, "Development of high-fidelity simulations of gas turbine combustors for sustainable aviation applications", awarded 128k Core-hours
3. DOE VTO's PACE program: high fidelity simulations of Sandia's DISI internal combustion engine

4. DOE AMO's HPC4EI programs: gas turbine film cooling flow and conjugate heat transfer in impinging jet flow

**COLLABORATORS (*PAST 5 YEARS INCLUDING NAME AND CURRENT INSTITUTION*)**

Muhsin Ameen (TAPS/ANL), Pinaki Pal (TAPS/ANL), Debolina Dasgupta (TAPS/ANL), Chao Xu (TAPS/ANL), Saumil Patel (CPS/ANL), Michael Joly (Raytheon), Carlos Pantano (USC), Paul Fischer (UIUC & MCS/ANL), Kenneth Christensen (IIT)

# Section 6: Software Applications and Packages

### Question #1

*Please list any software packages used by the project, and indicate if they are on open source or export controlled.*

### Application Packages

**Package Name**

Nek5000

**Indicate whether Open Source or Export Controlled.**

Open Source

**Package Name**

gslib

**Indicate whether Open Source or Export Controlled.**

Open Source

**Package Name**

Sundials/CVODE

**Indicate whether Open Source or Export Controlled.**

Open Source

**Package Name**

Cantera

**Indicate whether Open Source or Export Controlled.**

Open Source

**Package Name**

Zero-RK

**Indicate whether Open Source or Export Controlled.**

Open Source

# Section 7: Wrap-Up Questions

### Question #1

*National Security Decision Directive (NSDD) 189 defines Fundamental Research as "basic and applied research in science and engineering, the results of which ordinarily are published and shared broadly within the scientific community, as distinguished from proprietary research and from industrial development, design, production, and product utilization, the results of which ordinarily are restricted for proprietary or national security reasons." Publicly Available Information is defined as information obtainable free of charge (other than minor shipping or copying fees) and without restriction, which is available via the internet, journal publications, textbooks, articles, newspapers, magazines, etc.*

*The INCITE program distinguishes between the generation of proprietary information (deemed a proprietary project) and the use of proprietary information as input. In the latter, the project may be considered as Fundamental Research or nonproprietary under the terms of the nonproprietary user agreement. Proprietary information, including computer codes and data, brought into the LCF for use by the project - but not for generation of new intellectual property, etc., using the facility resources - may be protected under a nonproprietary user agreement.*

### Proprietary Information

**Are the proposed project and its intended outcome considered Fundamental Research or Publicly Available Information?**

Yes

**Will the proposed project use proprietary information, intellectual property, or licensing?**

No

**Will the proposed project generate proprietary information, intellectual property, or licensing as the result of the work being proposed?**

***If the response is Yes, please contact the INCITE manager, INCITE@doeleadershipcomputing.org, prior to submittal to discuss the INCITE policy on proprietary work.***

No

## Question #2

*The following questions are provided to determine whether research associated with an INCITE proposal may be export controlled. Responding to these questions can facilitate - but not substitute for - any export control review required for this proposal.*

*PIs are responsible for knowing whether their project uses or generates sensitive or restricted information. Department of Energy systems contain only data related to scientific research and do not contain personally identifiable information. Therefore, you should answer "Yes" if your project uses or generates data that fall under the Privacy Act of 1974 U.S.C. 552a. Use of high-performance computing resources to store, manipulate, or remotely access any national security information is prohibited. This includes, but is not limited to, classified information, unclassified controlled nuclear information (UCNI); naval nuclear propulsion information (NNPI); and the design or development of nuclear, biological, or chemical weapons or of any weapons of mass destruction. For more information contact the Office of Domestic and International Energy Policy, Department of Energy, Washington DC 20585, 202-586-9211.*

### Export Control

**Does this project use or generate sensitive or restricted information?**

No

**Does the proposed project involve any of the following areas?**

**i. Military, space craft, satellites, missiles, and associated hardware, software or technical data**

**ii. Nuclear reactors and components, nuclear material enrichment equipment, components (Trigger List) and associated hardware, software or technical data**

**iii. Encryption above 128 bit software (source and object code)**

**iv. Weapons of mass destruction or their precursors (nuclear, chemical and biological)**

No

**Does the proposed project involve International Traffic in Arms Regulations (ITAR)?**

No

## Question #3

*The following questions deal with health data. PIs are responsible for knowing if their project uses any health data and if that data is protected. Note that certain health data may fall both within these questions as well as be considered sensitive as per question #2. Questions regarding these answers to these questions should be directed to the centers or program manager prior to submission.*

**Health Data**

**Will this project use health data?**

No

**Will this project use human health data?**

No

**Will this project use Protected Health Information (PHI)?**

No

**Question #4**

*The PI and designated Project Manager agree to the following:*

**Monitor Agreement**

**I certify that the information provided herein contains no proprietary or export control material and is correct to the best of my knowledge.**

Yes

**I agree to provide periodic updates of research accomplishments and to acknowledge INCITE and the LCF in publications resulting from an INCITE award.**

Yes

**I agree to monitor the usage associated with an INCITE award to ensure that usage is only for the project being described herein and that all U. S. Export Controls are complied with.**

Yes

**I understand that the INCITE program reserves the right to periodically redistribute allocations from underutilized projects.**

Yes

# Section 8: Outreach and Suggested Reviewers

### Question #1

*By what sources (colleagues, web sites, email notices, other) have you heard about the INCITE program? This information will help refine our outreach efforts.*

### Outreach

**By what sources (colleagues, web sites, email notices, other) have you heard about the INCITE program? This information will help refine our outreach efforts.**

ALCF

### Question #2

### Suggested Reviewers

**Suggest names of individuals who would be particularly suited to assess the proposed research.**

Dr. Jacqueline O'Connor (Pennsylvania State University)

# Section 9: Testbed Resources

### Question #1

*The ALCF and OLCF have test bed resources for new technologies, details below. If you would like access to these resources to support the work in this proposal, please provide the information below. (1 Page Limit)*

*The OLCF Quantum Computing User Program is designed to enable research by providing a broad spectrum of user access to the best available quantum computing systems, evaluate technology by monitoring the breadth and performance of early quantum computing applications, and Engage the quantum computing community and support the growth of the quantum information science ecosystems. More information can be found here: [https://www.olcf.ornl.gov/olcf-resources/compute-systems/quantum-computing-user-program/quantum-computing-user-support-documentation](https://www.olcf.ornl.gov/olcf-resources/compute-systems/quantum-computing-user-program/quantum-computing-user-support-documentation).*

*The ALCF AI Testbed provides access to next-generation of AI-accelerator machines to enable evaluation of both hardware and workflows. Current hardware available includes Cerebras C-2, Graphcore MK1, Groq, Habana Gaudi, and SambaNova Dataflow. New hardware is regularly acquired as it becomes available. Up to date information can be found here: [https://www.alcf.anl.gov/alcf-ai-testbed](https://www.alcf.anl.gov/alcf-ai-testbed).*

**Describe the experiments you would be interested in performing, resources required, and their relationship to the current proposal. Please note, these are smaller experimental resources and a large amount of resources are not available. Instead, these resources are to explore the possibilities for these technologies might innovate future work. This request does not contribute to the 15-page proposal limit.**

Testbed.pdf
The attachment is on the following page.

We are not planning to need access to the ALCF and OLCF testbed resources as part of this proposal.