# 2023 INCITE Proposal Submission
## Proposal

**Title: Novel high-fidelity moment closures for polydisperse multiphase turbulent flows**

**Principal Investigator: Lucian Ivan**

**Organization: Canadian Nuclear Laboratories**

**Date/Time Generated: 6/17/2022 10:27:51 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


**First Name**

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**Question #2**

**Co-PI (s)**

**First Name**

James G.

**Last Name**

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**Organization**

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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**

Ashlea Colton

**Institutional Contact Phone**

613-602-3192

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# Section 2: Project Information

**Question #1**

*Select the category that best describes your project.*

**Research Category**

Engineering: Fluids and Turbulence

**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**

The COVID-19 pandemics exposed the need to improve the physics-based models for describing how carrier aerosols of respiratory viruses are transported. Capability demonstration of advanced models is necessary for proving fitness in mitigating future pandemics. Leveraging of these advanced capabilities could also elucidate fundamental aspects about the nature of turbulence.

# 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.**

No

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

N/A

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

N/A

# 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**

1,000,000

**Storage (TB)**

30

**Off-Line Storage (TB)**

N/A

**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 Xe) Resource Request – 2023**

**Question #10**

**ALCF Aurora (Intel Xe) Resource Request – 2024**

**Question #11**

**ALCF Aurora (Intel Xe) Resource Request – 2025**

**Question #12**

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

**Funding Sources**

**Funding Source**

Atomic Energy of Canada Limited (AECL) Federal Nuclear Science and Technology (FNST) at Canadian Nuclear Laboratories

**Grant Number**

N/A

**Funding Source**

Natural Science and Engineering Research Council of Canada (NSERC) Discovery Grant

**Grant Number**

RGPIN-2020-06295

**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.**

proposal.pdf
The attachment is on the following page.

## PROJECT EXECUTIVE SUMMARY

**Title (*80 characters max; strictly enforced*)**: Novel high-fidelity moment closures for polydisperse multiphase turbulent flows

**PI and Co-PI(s)**: Lucian Ivan and James G. McDonald

**Applying Institution/Organization**: Canadian Nuclear Laboratories and University of Ottawa

**Resource Name(s) and Number of Node Hours Requested**: 1,000,000 node-hours

**Amount of Storage Requested**: 30 Tb

**Executive Summary (*May use the remainder of page*):**

The transmission of pathogen-laden particles generated by respiratory events has been identified as the main spreading route for SARS-CoV-2 infection in a variety of indoor and outdoor environment settings. High-fidelity computational tools that can provide an improved prediction and uncertainty quantification of pathogen-laden aerosol dispersion are instrumental in performing pathogen risk assessment, designing improved ventilation systems, and/or devising mitigation and prevention strategies for pandemic readiness. The first scientific goal is to levarage recent advances in the development of polydisperse Gaussian-moment models (PGM) to improve the understanding and prediction accuracy of bioaerol dispersion.

Despite various successful computational models that have been proposed for the simulation of multiphase turbulent flows based on both Lagrangian and Eulerian formulations, available models for particle-laden flows are still confronted with difficulties. This is especially true for transitional flow regimes such as those encountered in the dispersion of pathogen-laden aerosols which exhibits transition from granular to dilute regimes with the distance from the infected subject. Although extremely dilute flows can be described efficiently using particle-tracking methods, i.e., Lagrangian approaches, the computational cost of these methods increases significantly as the number of particles becomes large and/or the number of sampling experiments for achieving statistical significance increases (e.g., sample from the distribution of droplet sizes in a cough). Alternatively, the PGM model recently proposed is a field-based technique in the framework of moment closures of the Boltzmann equation. In addition to extending the region of physical validity to non-equilibrium, transition-regime particle-laden flows, the PGM can be expected to be more computationally affordable for flows exhibiting a large number of particles, such as those associated with complex situations (e.g., long duration monitoring of venues with multiple infection sources). This project would be the first practical large-scale application of moment-closure methods to the prediction of polydisperse multiphase flows.

A secondary scientific goal in the research is to perform a first of its kind assessment of moment-based methods for the study of turbulence. Towards this goal, we will perform direct numerical simulation (DNS) studies with moment-based methods for the Taylor-Green benchmark case. This will pave the way towards investigating the potential thermodynamic non-equilibrium effects at the smallest scales of the turbulence spectrum. Traditionally, it is assumed that turbulence is a fully continuum phenomenon fully described by the continuum Navier-Stokes equations. The use of a moment method, which directly tracks non-equilibrium effects, could uncover deviations from the classical theory. This possible fundamental finding would have huge implications in the theory of turbulence.

The two scientific goals of this project hold the promise of leading to fundamental advances of importance to myriad flows, but the resolutions required to produce resolved solutions are only possible with resources provided by the INCITE program.The techniques demonstrated in this project will apply to other areas of practical application such as prediction of radionuclides dispersion following nuclear events, dispersion of pollutants in the atmosphere, and spray modelling, just to name a few.

# PROJECT NARRATIVE

## 1 SIGNIFICANCE OF RESEARCH

### Significance of Scientific Goal 1

As of February 19, 2022, i.e., more than two years after the SARS-CoV-2 virus has spread across the world, the World Health Organization (WHO) recorded over four hundred million confirmed cases and almost six million deaths due to COVID-19 [1]. SARS-CoV-2, the virus that causes COVID-19, spreads from an infected person to others through respiratory droplets and aerosols when an infected person breathes, coughs, sneezes, sings, shouts, or talks. The droplets vary in size, from large droplets that fall to the ground rapidly (within seconds or minutes) near the infected person, to smaller droplets, sometimes called aerosols, which linger in the air [2], especially in indoor spaces, for much longer periods of time (e.g., hours), thus increasing the risk of contagion. Observational studies in indoor environments (e.g., restaurants, public transit) point to a link between ventilation rates and virus transmission, but there are no established requirements on ventilation protocols. It can be assumed that aerosol concentrations in indoor environments should be kept low to minimize the potential risk of virus transmission. However, there is limited knowledge on the aerosol concentrations in different types of indoor environments (e.g., fitness gyms, department stores, offices, hospitals) [3].

### Significance of Scientific Goal 2

The models being proposed for the modern treatment of aerosol transport problems derive from the kinetic theory of gases. When applied to purely gaseous flows they offer additional modelling accuracy in regimes in which the traditional continuum models provide incorrect predictions. One phenomena of fundamental importance to myriad flows is the presence of turbulence. The traditional understanding for the past century is that all turbulence scales occur in a continuum regime. However, this established assumption has been more recently revisited in relation to certain flows, and scale analysis arguments suggest that non-continuum effects could play an important role at the smallest scales. The novel models investigated in this project pave the way to perform studies that could elucidate the importance of such non-equilibrium effects in canonical turbulence situations. The clarification of this important question could lead to fundamental changes in the understanding of turbulence.

## 1.1 Scientific Goal 1: Improve prediction of virus-laden aerosols using a Gaussian-moment model

### *1.1.1 Background*

Although general guiding principles have been formulated to mitigate the exposure risk (e.g., wearing a facemask, keeping two meters or six feet apart from people), it has been pointed out [2] that transmission is more complex in reality and distancing rules need to take into account multiple factors including viral load, ventilation, type of activity, environment settings, and wearing of PPE (personal protective equipment). Despite the increased scientific attention received by airborne transmission in light of the ongoing SARS-CoV-2 (COVID-19) pandemic, there is still a lack of generally applicable, physics-based modelling tools to assess the effectiveness of safety measures and 'air disinfection' methods [4] in a variety of settings. Although the COVID-19 risk of severe disease and death have dramatically reduced lately, improving the understanding of airborne transmission of SARS-CoV-2 virus is still relevant for the current pandemic and likely more importantly, preparing for future ones. Thus, modelling tools developed from present state-of-the-art approaches are expected to contribute to devising mitigation strategies for reducing the risk of further

spread of the SARS-CoV-2 virus, more virulent future strains, as well as as assisting in future outbreaks or pandemics due to other pathogens.

Since specific airflow patterns are important in determining risk of exposure and transmission [2], physics-based modelling approaches for predicting airborne transmission have to resolve a variety of complex physical phenomena associated with the ejection and dispersion of saliva droplets in an airflow driven by air conditioning, ventilation, occupancy of the space, air recirculation, and filtration. Depending on how violent the aerosol-generating procedure is, published data [5] have suggested that a single sneeze can generate $\mathcal{O}(10^4)$ or more droplets, with velocities upwards of $20\,\mathrm{m\,s^{-1}}$. Coughing generates 10–100 times fewer droplets than sneezing, with velocities of approximately $10\,\mathrm{m\,s^{-1}}$, but even talking can generate approximately 50 particles per second. Measured droplet sizes range over four orders of magnitude, from $\mathcal{O}(0.1)$ to $\mathcal{O}(10^3)$ μm, and they follow a distribution which can be fit with a log-normal curve in particle diameter [6]. It follows that the majority of aerosols in violent expiratory events, about 97% of the total number, are less than one micron in size and form contaminated aerosols which can remain suspended in the surrounding air after all liquid has evaporated. Aerosol agglomeration (i.e., aerosols colliding to create larger sizes) and deposition mechanisms (e.g., gravitational settling has stronger effect on larger aerosols), aerosol evaporation, along with more global parameters like ventilation rates and temperatures, dictate the time evolution of the airborne concentrations in a particular setting. Airflow within the room, generated by forced convection (i.e., HVAC or fans) or free convection (buoyancy induced by temperature differences) will transport the aerosols between people. Finally, the decay (die off of the virus) will determine the viability of the transported pathogen to infect upon coming into direct contact with the mucous membranes of another person's nose, mouth or eyes, or by being inhaled into their nose, mouth, airways and lungs.

### *1.1.2 Proposed Approach*

From a fluid-dynamics perspective, describing the transmission of virus-laden aerosol particles related to respiratory virus infections is equivalent to modelling a multiphase particle-laden flow. The disperse phase is made up of the relatively small virus-laden saliva droplets that are suspended in a continuously connected carrier phase representing the airflow due to the cough/sneeze jet and the surrounding air currents. The flow is said to be polydisperse since the constituent particles, which can be assumed of spherical shape, exhibit a range of equivalent aerodynamic diameters. Moreover, the particle-laden flow is either dilute or granular if the mass fraction of the disperse phase is small or large, respectively. Thus, the polydisperse multiphase particle-laden flow encountered in aerosol transmission would generally be granular near the release source, i.e., the infected person, and transition to a dilute regime further away. A few other examples of applications of particle-laden flows include particle separators, hydraulic and pneumatic conveyors, fluidization in combustion processes, fluidized bed reactors, settling tanks, and dispersion of pollutants in the atmosphere.

Various computational models have been developed for the simulation of multiphase flows based on both Lagrangian and Eulerian formulations, e.g., [7, 8, 9, 10, 11]. Despite these many successes, it can be argued that there is still a range of flow conditions for which the available models are confronted with difficulties. In particular, no attractive method exists for particle-laden flow regimes, as determined by the spatial and temporal variation of the mass fraction and flow Stokes number, between the traditional continuum and free-particle limits. Extremely dilute flows can be described efficiently using particle-tracking methods, i.e., Lagrangian approaches, while a more computationally affordable formulation for granular or "continuous" regimes is provided by field-based (Eulerian) methods. More specifically, Lagrangian methods can provide predictive simulations for a vast range of mass fractions but they bring added computational expense, as well as increased complexities associated with the computational load balancing on parallel machines, as the number of particles becomes large. This added computational cost renders the computations unnecessarily

expensive for high mass fractions. Alternatively, Eulerian methods rely on partial differential equations (PDEs) for the evolution of field variables and, therefore, can be expected to be more computationally affordable for flows exhibiting a large number of particles.

Recent studies have used numerical simulations to analyze various aspects of the jet flow and the accompanying aerosol transport for flow containing pathogen-carrying droplets of varying sizes (see for instance [12, 13, 14, 15]). The dispersed saliva droplets are almost exclusively tracked as individual Lagrangian particles with only a few exceptions. Kumar and Lee [13] have modelled the virus-laden droplets as two different phases: a continuous phase governed by the Navier-Stokes equations (i.e., a Newtonian fluid) for the small size droplet nuclei and a discrete phase for large size droplets. Although relatively successful, these recently performed simulations of micro-infectious droplets rely on tracking samples of individual droplets from the droplet characteristics distribution, and determining the spatial and temporal statistical distribution of the particles based on an ensemble of simulations. Therefore, to get statistically converged predictions necessary for risk assessment and countermeasures strategies investigation, such approaches would become computationally intensive or even impractical for long monitoring periods of large indoor environments exhibiting multiple infected individuals, such as public places, transit, offices, classrooms, nursing homes, and hospital rooms.

Unfortunately, traditional Eulerian models can suffer from modelling artifacts that can render them invalid in certain situations, which include the conditions present in aerosol transmission. In particular, these gas-dynamic-like models rest on a continuum assumption and retain little or no information regarding the microscopic, particle nature of the disperse phase. Although these methods have been extremely successful in the prediction of particle flows that remain tightly coupled to the background fluid, they become inaccurate for transition-regime predictions. For instance, the most common field-based models do not allow for the crossing of streams of non-interacting particles [16, 17], a deficiency which stems from the common assumption that all particles at a location in space share the same velocity.

The current work is concerned with a new Eulerian formulation for the modelling of multiphase particle-laden flows when particles are differentiated by a set of distinguishable properties such as size, temperature, or viral load. Recently, Forgues *et al.* [18] have proposed a general moment-closure-based framework that is accurate and efficient for transition-regime particle-laden-flow prediction. In particular, the recently proposed polydisperse Gaussian-moment model (PGM) described in [18] is an efficient PDE-based method with validity spanning the continuum and transition regimes and a computational cost that is comparable to traditional continuum-regime methods. The model is described by fifteen first-order hyperbolic balance laws that provide an Eulerian treatment for higher-order statistics describing a particle phase in a background flow. Predictive capabilities of the model investigated in [18] have been demonstrated for one-dimensional (1D) flows when particle drag, buoyancy, and gravitational acceleration are considered. The PGM formulation is an extension of the well-known ten-moment maximum-entropy model from rarefied gas dynamics and provides a direct treatment for local variances and covariances between all particle properties and velocities. This statistical information is not commonly available or utilized in traditional Eulerian methods and holds the promise of improved modelling accuracy at reduced computational cost.

In our previous work [18], we have investigated a formulation based on a log-normal distribution of particle size, as there are many processes in which a log-normal distribution of the particle diameters is encountered, including the human cough [19]. However, the original log-normal version of the model does not correctly recover the settling rates for particles in a quiescent atmosphere, which prompted the investigation of a formulation which assumes that particle surface area follows a normal distribution. In contrast, the surface-area-based version of the model [20, 21] is designed to recover this settling rate ex-

actly. Moreover, all PGM variants have now been implemented in a modern, massively parallel, three-dimensional (3D), solution-adaptive computational framework that provides up to third-order accuracy based on a discontinuous-Galerkin-Hancock (DGH) numerical scheme [22, 23].

Preliminary studies to demonstrate the validity of the PGM approach for conditions resembling those of airborne transmission have been performed on ALCF Theta KNL system under a Director's Discretionary (DD) allocation (30,000 node-hours). Additionally, a formulation for the effect of evaporation has also been developed. The high-resolution aerosol simulations performed on this system using the recently-proposed surface-weighted polydisperse Gaussian-moment method (SW-PGM) are included in a conference submission [20] and into a journal article manuscript [21]. Validation and application to a range of practical conditions require to generate resolved solutions for a large number of conditions. An allocation of petascale resources would allow us to perform these studies in a timely fashion, which in turn will provide the validation of a novel model for application to a wide range of polydisperse multiphase flows.

Among many potential applications for these Eulerian models, the atmospheric dispersion of aerosols, of virulent or a different contaminant type nature, is a particular example in which such transitional regimes (e.g., from a dense granular to a dilute flow) occur due to the presence of very large domains. Therefore, there is a wider class of multiphase-flow applications to which the PGM formulation and the computational tools developed as part of this proposal can prove extremely relevant, such as modelling radionuclides dispersion for emergency response and preparedness (e.g., nuclear accidents and/or malicious attacks) and spray atomization models, just to name a few.

## 1.2 Scientific Goal 2: Investigate existence of non-continuum effects at Kolmogorov scale for turbulent flows

The carrier phase of the multiphase flow encountered in airborne transmission is often in a turbulent regime. Various approaches have been already considered for its modelling, which include Reynolds-average turbulence models [13], large-eddy simulation (LES) techniques [14], and, depending on the situation, simpler turbulent jet-type approximations [24, 25]. In our work to date, the latter approaches have also been considered as well as turbulence models derived from hyperbolic moment-closure formulations [26], which is in contrast to the traditional, hydrodynamic-type turbulence models based on the Navier-Stokes equations.

A key advantage of describing viscous flows with moment-based models derived from gaskinetic theory using an entropy-maximization formulation (see details in Sect. 2.1) is that it extends the model validity beyond the continuum regime of the fluid flow. This novel capability of our modelling framework paves the way to investigate essential and long-lasting questions related to turbulent flows: can there be non-continuum effects present at Kolmogorov scale for turbulent flows, which are the smallest length and time scales of the turbulence at which the dissipation occurs? If so, how relevant is it that these effects are accounted for? This is the focus of our second scientific goal.

Turbulence is almost exclusively studied at the hydrodynamic (continuum) level. Molecular-level simulations of turbulence have received little, if any, attention to date because the molecular scales and the turbulent scales are considered to be many orders of magnitude apart, and, as a result, molecular turbulence simulations have been heretofore considered to be physically unnecessary and computationally intractable. However, there are cases of practical interest [27, 28] in which the Kolmogorov length and time scales can be within one-to-two orders of magnitude of the mean free path and the mean collision time. For a high-speed gas flow with a turbulent Mach number and a turbulent Reynolds number, a scaling analysis estimates that the ratio of the Kolmogorov length scale to the mean free path and the ratio of the Kolmogorov time scale to the mean collision time is approximately 10 and 100, respectively, under certain conditions [28]. In such

cases, studying turbulence and energy exchange at the molecular level may offer new physical insights.

Recently, Gallis *et al.* [27] provided the first demonstration that molecular-level methods based on gas kinetic theory and molecular chaos can simulate turbulence and its decay, by applying a direct simulation Monte Carlo (DSMC) method to simulate the Taylor-Green vortex flow [29]. Despite its relative success for lower Reynolds number cases, DSMC is an expensive technique for resolving phenomena from molecular to hydrodynamic (continuum) length scales in gas flows as it uses probabilistic Monte Carlo simulation to solve the Boltzmann equation. Alternatively, the moment-based methods used in our work lead to a set of first-order hyperbolic balance laws with stiff relaxation source terms for the description of turbulent viscous, compressible fluid flow, that extends over the continuum limit of flow regimes into the transitional domain [30]. Despite offering a viable alternative to the Navier-Stokes equations, moment-based methods do not appear to have been considered for the direct numerical simulation (DNS) of turbulent flow. Thus, the investigation pursued here is novel and a first-of-a-kind in its approach.

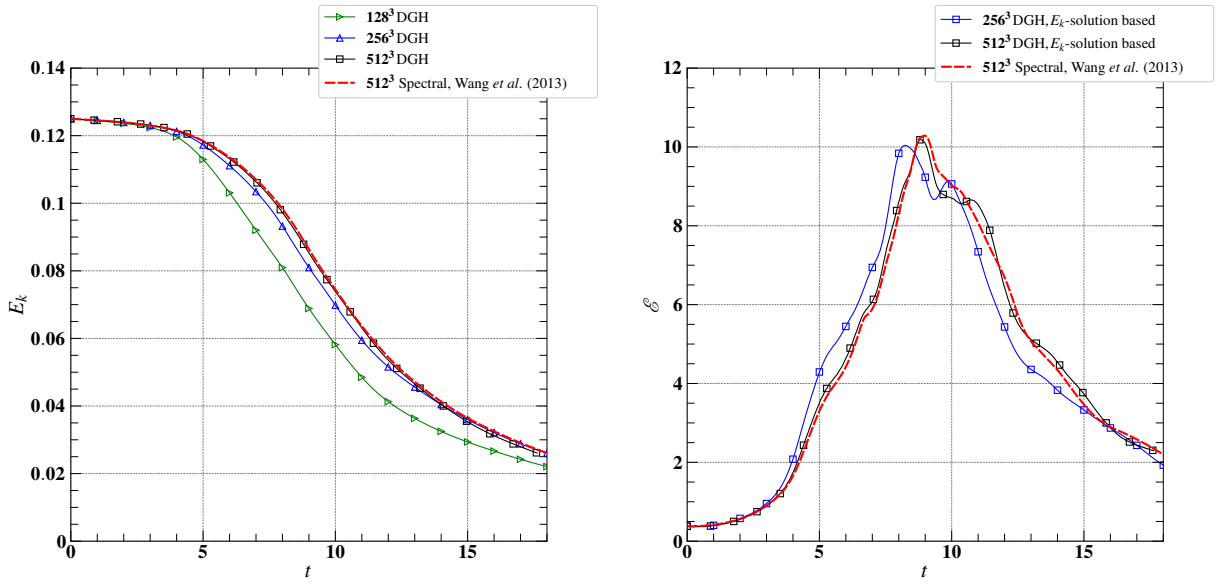
A key enabler in this work for performing novel DNS studies with the hyperbolic ten-moment model [31] (see Sect. 2.1.1 for details) has been the development and implementation of a recently proposed third-order, coupled space-time DGH method with an efficient locally implicit treatment for stiff source terms [23]. Computational studies using the benchmark Taylor-Green vortex problem [29] have been performed on ALCF Theta KNL system to investigate the predictive capabilities of the hyperbolic moment-model for DNS of turbulent flow. Figure 1 depicts a recent result for this problem, in which the initial condition of the compressible, diatomic perfect gas flow leads to a transition to turbulence followed by subsequent decay. The predicted temporal evolution of the kinetic energy, $E_k$, and enstrophy, $\mathscr{E}$, on a sequence of uniformly refined Cartesian meshes is depicted in Fig. 1(a) and (b), respectively. Note that the enstrophy can be obtained using the solution gradient or its relationship to the temporal rate of change of $E_k$ [29]. The plots reveal that the DGH predictions approach the reference solution as the mesh is refined, but the prediction on the most refined grid does not fully agree with the continuum result. Although no definite conclusion can be made about the numerical convergence of the result on the finest resolution, an inspection of the Kolmogorov scale for this problem [32] reveals that it is on the order of the cell length. Furthermore, the Knudsen number of that scale is approximately 0.008 which corresponds to regimes at which non-equilibrium effects begin to be observed. Additional high-resolution studies of this and other relevant cases are planned to be carried out as part of this proposal to validate the proposed approach. Moreover, postulated situations for non-continuum effects [28] will be investigated. Considering the large number of computational elements required for resolving the solution features, even with high-order accuracy schemes, (e.g., on the order of 100's to 1,000's of million of grid points), these studies require petascale computing capabilities.

## 2 RESEARCH OBJECTIVES AND MILESTONES

This section provides a brief description of the Gaussian-moment-based models developed to support this research and the numerical techniques employed for computational studies. The project milestones for achieving the aforementioned two scientific goals (Sect. 1.1 and 1.2 ) are also defined and discussed at the end of the section.

### 2.1 The Gaussian-Moment Method for Gases and Polydisperse Multiphase Flow

Moment closures follow from the kinetic theory of gases [34]. In this theory, the particle nature of a gas is not ignored, however, the individual evolution of each atom or molecule is not directly tracked. Rather, a distribution function, $\mathscr{F}(x_i, v_i, t)$, is defined which gives the phase-space density of particles of a single-species gas at a position, $x_i$, with velocity, $v_i$, at a time, $t$. As the situation of a polydisperse multiphase flow is similarly composed of a large number of particles, a similar technique can also be used for these




**(a) The kinetic energy, $E_k$.** **(b) The enstrophy, $\mathscr{E}$.**

**Fig. 1. Plot of the predicted kinetic energy and enstrophy by the ten-moment model along with the reference NS-based solution from Jacobs *et al.* [33] (verified against Wang *et al.* [29]).**

situations [9, 35, 10, 11, 36]. However, the particles of a multiphase flow are rarely identical. Rather, they can be distinguished by variation in size, temperature, chemical content, or any other important property. To take this into account in the kinetic description, the distribution function is extended into a new dimension for each distinguishing property considered, $\mathscr{F}(x_i, v_i, \Upsilon_\mu, t)$. This new distribution function gives the density of particles in an expanded phase space at $x_i$, $v_i$ and $t$ with distinguishing properties of interest described by the entries of the vector $\Upsilon_\mu$.

Traditional macroscopic variables can be computed by taking moments of $\mathscr{F}$. This is done by multiplying the distribution function by an appropriately chosen weight and integrating over all velocity space. For example, the spacial number density of particles is given by

$$n(x_i,t) = \int_{\infty} \mathscr{F}\, \mathrm{d}v_i\, \mathrm{d}\Upsilon_\mu = \langle \mathscr{F} \rangle \,.$$

Here, the weight is simply taken as the constant of unit value, and the compact notation, $\langle\cdot\rangle$, denotes integration over all three dimensions of velocity space and all dimensions of chosen distinguishing variables. Other commonly used moments are

$$n u_i = \langle v_i \mathscr{F} \rangle \,, \qquad n\Theta_{ij} = \langle c_i c_j \mathscr{F} \rangle \,, \qquad n Q_{ijk} = \langle c_i c_j c_k \mathscr{F} \rangle \,,$$
$$n\Psi_{i\mu} = \langle v_i \left(\Upsilon_\mu - \overline{\Upsilon}_\mu\right) \mathscr{F} \rangle \,, \qquad n\Psi_{\mu\mu} = \left\langle v_i \left(\Upsilon_\mu - \overline{\Upsilon}_\mu\right)^2 \mathscr{F} \right\rangle \,, \qquad n\overline{\Upsilon}_\mu = \langle \Upsilon_\mu \mathscr{F} \rangle \,.$$

Here, $u_i$ is the average particle velocity at a point and time, and $\overline{\Upsilon}_\mu$ is the local average value of the $\mu$th distinguishing variables. This allows the difference between individual particle velocities and the local average to be defined as $c_u = v_i - u_i$. The variance-covariance tensor, $\Theta_{ij}$, describes the spread of particle velocities and the correlation between individual components of the particle velocities, $\Psi_{i\mu}$ is the covariance between the $i$th component of a particle velocity and the $\mu$ distinguishing variable, while $\Psi_{\mu\mu}$ is the local

variance of the $\mu$th distinguishing variable. The third-order tensor, $Q_{ijk}$, is the generalized skewness tensor and represents asymmetries of the distribution function. Moments of arbitrarily high order can be taken, however, the interpretation of their meaning becomes harder and harder.

One can immediately see the potential for models in this framework to directly consider and respond to high-order statistics of particle states that are not considered in traditional models. This extra information can lead to efficient models that are more accurate and do not suffer from modelling artifacts present in classical Eulerian treatments.

The evolution of the particle distribution function is governed by a kinetic equation,

$$\frac{\partial \mathscr{F}}{\partial t} + v_i \frac{\partial \mathscr{F}}{\partial x_i} + \frac{\partial}{\partial v_i}\left(a_i \mathscr{F}\right) + \frac{\partial}{\partial \Upsilon_\mu}\left(\Phi_\mu \mathscr{F}\right) = S. \tag{1}$$

Here, $a_i$ is the particle acceleration due to effects such as drag or external fields. The variable, $\Phi_\mu$, is the rate of change of $\Upsilon_\mu$ for a particle. For example, if the variable of interest is particle size, $\Phi_\mu$ could be the rate of size change due to evaporation or other effects. Finally, the local source term on the right-hand side is chosen to be appropriate for the situation of interest. For example, if the right-hand side is taken to be the Boltzmann collision integral and the particles are assumed to be indistinguishable (there are no variables, $\Upsilon_\mu$), Eq. (1) becomes the well-known Boltzmann equation of gas dynamics [37]. If the distinguishing variables are taken to be particle size and temperature, it becomes the Williams spray equation [38].

Equation (1) is extremely flexible and can be adapted to model a very wide range of situations, however it is extremely high dimensional. The equation exists in three space dimensions, three velocity dimensions, a chosen number of dimensions for the particle distinguishing characteristics, and time. Any solution through a direct discretization would be extremely expensive and limited to trivially small problems. Fortunately, a lower-dimensional equation can be derived for a given macroscopic statistical moment of the $\mathscr{F}$. For example, given a weight function, $W$, that corresponds to an arbitrary moment, $\langle W\mathscr{F}\rangle$, a moment of Eq. (1) gives

$$\frac{\partial}{\partial t}\langle W\mathscr{F}\rangle + \frac{\partial}{\partial x_i}\langle v_i W\mathscr{F}\rangle = -\left\langle a_i \mathscr{F}\frac{\partial W}{\partial v_i}\right\rangle - \left\langle \Phi_\mu \mathscr{F}\frac{\partial W}{\partial \Upsilon_\mu}\right\rangle + \langle WS\rangle\,. \tag{2}$$

For many situations, all terms on the right-hand side of Eq. (2) can be evaluated in closed form and yield algebraic expressions. However, on the left-hand side, one sees that the time evolution of an arbitrary moment will always depend on the divergence in space of a moment of one order higher. This will lead to an infinite set of coupled equations and is obviously impractical.

Any technique used to close the infinite set of equations resulting from Eq. (2) is known as a *moment closure*. The most popular way of doing this is by restricting the allowed form of $\mathscr{F}$ to have a prescribed form in terms of a finite number of closure coefficients. In doing so, the number of degrees of freedom is restricted and the moment equations naturally close.

Though many techniques exist for closing the form of $\mathscr{F}$, in this work, an entropy maximization principle is used [39, 40, 41]. In this method, a set of moments of interest are chosen, then $\mathscr{F}$ is restricted to be whatever has the highest entropy while being consistent with the known moments. Moment closures of this type yield expanded sets of first-order hyperbolic balance-laws for the evolution of the chosen moments.

### *2.1.1 The Ten-Moment Gaussian Model of Gas Dynamics*

One successful member of the maximum-entropy hierarchy for gases is the ten-moment, or Gaussian, moment model. This model results from choosing number density, local average velocity, and the velocity

variance-covariance tensor as the moments of interest. The maximum-entropy theory leads to a distribution function of the form

$$\mathscr{F}_{\mathrm{G}} = \frac{n}{(2\pi)^{\frac{3}{2}}(\det\Theta_{ij})^{\frac{1}{2}}} \exp\left(-\frac{1}{2}\Theta_{ij}^{-1}c_i c_j\right). \tag{3}$$

Insertion of this assumed form into Eq. (2) gives a set of three tensor equations for ten independent fields,

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_k} n u_k = 0\,, \tag{4}$$

$$\frac{\partial}{\partial t} n u_i + \frac{\partial}{\partial x_k} n(u_i u_k + \Theta_{ik}) = 0\,, \tag{5}$$

$$\frac{\partial}{\partial t} n\left(u_i u_j + \Theta_{ij}\right) + \frac{\partial}{\partial x_k} n\left(u_i u_j u_k + u_i\Theta_{jk} + u_j\Theta_{ik} + u_k\Theta_{ij}\right) = S_G\,. \tag{6}$$

This first-order hyperbolic model for viscous compressible gases can be seen as an alternative to the compressible Navier-Stokes equations. In fact, by allowing for anisotropic temperatures, the ten-moment model can remain accurate for significant departures from local thermodynamic equilibrium, in cases for which the Navier-Stokes equations lose validity. This model has proven successful in predictive viscous flows both in and out of thermodynamic equilibrium [42, 43, 44, 45]. In addition to being accurate and efficient, the first-order nature of the resulting equations has been shown to make numerical solutions less sensitive to grid quality [46]. This is especially advantageous for practical situations with complex geometry for which high-quality grid generation is very difficult.

### *2.1.2 The Fifteen-Moment Polydisperse Gaussian Moment Model*

The ten-moment model, Eq. (4)–(6), was originally derived for a monatomic gas, however, it can also be used in its original form for the particle phase of monodisperse flow of identical particles [36]. Only the algebraic source terms on the right-hand side need be changed. However, by extending the distribution function into an extra dimension corresponding to some measure of particle size, the polydisperse Gaussian moment model (PGM) can be found [18]. In the original PGM model, the particles are differentiated by size and the logarithm of the diameter, $\ln d$, is chosen as the measure. This leads to a log-normal distribution of particle sizes, which was experimentally observed in the application of interest here [6]. In this model, the ten-moment equations shown above are supplemented with a field for the average $\ln d$, the covariance of $\ln d$ with $v_i$, and the local variance of $\ln d$. This robustly hyperbolic model proved accurate for several flows of interest. However, it fails to recover the correct statistics of particles settling in a quiescent atmosphere.

More recently, a new version of the PGM has been derived taking the particle surface area as the measure of

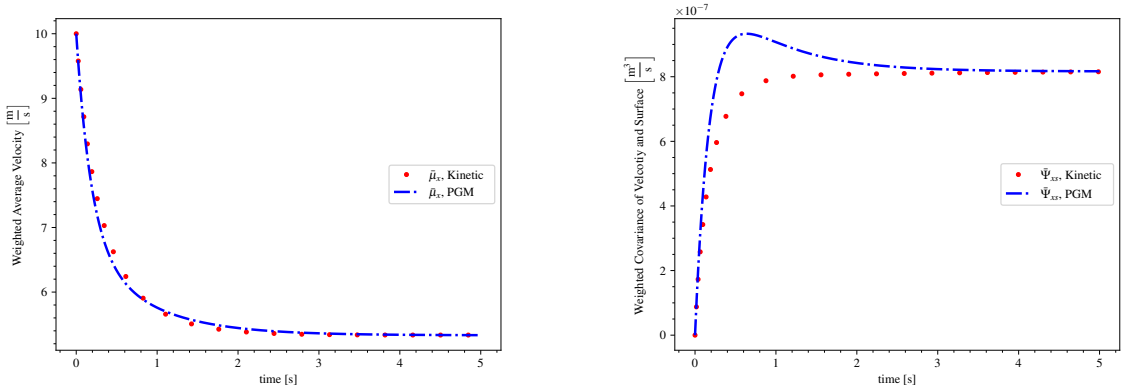



**Fig. 2. Space homogeneous settling particles**

particle size. Again, the resulting moment system comprises fifteen equations,

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_\alpha} n\mu_\alpha = S^{(1)}, \tag{7}$$

$$\frac{\partial}{\partial t} n\mu_i + \frac{\partial}{\partial x_\alpha} n(\Psi_{i\alpha} + \mu_i\mu_\alpha) = S_i^{(2)}, \tag{8}$$

$$\frac{\partial}{\partial t} n\left(\Psi_{ij} + \mu_i\mu_j\right) + \frac{\partial}{\partial x_\alpha} n\left(Q_{ij\alpha} + \mu_i\Psi_{j\alpha} + \mu_j\Psi_{i\alpha} + \mu_\alpha\Psi_{ij} + \mu_i\mu_j\mu_\alpha\right) = S_{ij}^{(3)}, \tag{9}$$

$$\frac{\partial}{\partial t} n\sigma + \frac{\partial}{\partial x_\alpha} n\left(\Psi_{\alpha s} + \mu_\alpha\sigma\right) = S^{(4)}, \tag{10}$$

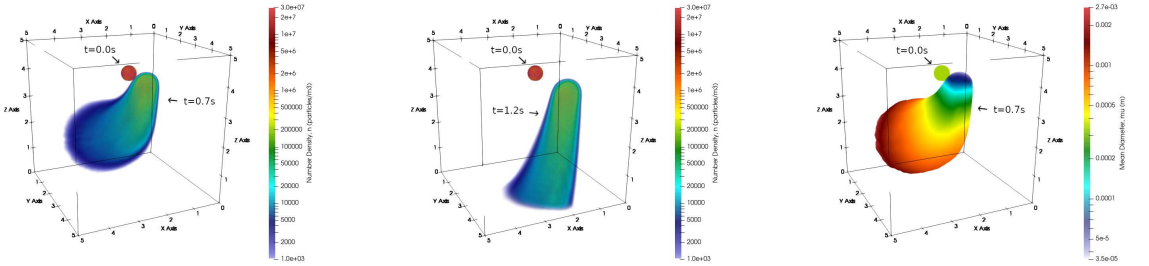
$$\frac{\partial}{\partial t} n(\Psi_{is} + \mu_i\sigma) + \frac{\partial}{\partial x_\alpha} n\left(Q_{i\alpha s} + \mu_i\Psi_{\alpha s} + \mu_\alpha\Psi_{is} + \sigma\Psi_{i\alpha} + \mu_i\mu_\alpha\sigma\right) = S_i^{(5)}, \tag{11}$$

$$\frac{\partial}{\partial t} n(\Psi_{ss} + \sigma^2) + \frac{\partial}{\partial x_\alpha} n\left(Q_{iss} + 2\sigma\Psi_{\alpha s} + \mu_\alpha\Psi_{ss} + \mu_\alpha\sigma^2\right) = S^{(6)}. \tag{12}$$

Here, $\sigma$ is the local average value of the surface area of the particles. The algebraic terms on the right-hand side can be chosen to include effects such as drag, gravity, buoyancy, evaporation, and effects of a turbulent background flow. By taking surface area as the measure of particle size, the model is proven to recover all steady-state statistics of settling particles exactly. This can be seen in Figure 2 which shows the statistical evolution of a space-homogeneous cloud of particles evolving from an initial state to a terminal settling state. Both the surface-weighted average velocity and covariance between the surface area and particle velocity are shown. Though the covariance undergoes a small modelling error in the transient, both statistics settle to a steady-state value in agreement with the exact solution. The positive value of the shown covariance correctly indicates that particles with large surface areas have higher terminal velocities.

As a demonstration of this model's ability to predict the dispersal of particles following a cough or sneeze, Figure 3 shows the dispersion of a spherical puff of polydisperse water droplets released with a range of initial velocities, having an initial mean velocity in the positive $x$ direction, into an ambient environment. Due to interaction with a transverse air current in the positive $y$ direction, the puff moves diagonally, with larger particles falling more quickly due to gravity and drag. Figure 3(c) provides information about the location of smaller and larger particles as depicted by lower and higher values of mean diameter, respectively. This is enabled by the direct treatment of the local covariance between particle size and velocity.

The use of moment-based methods that directly track high-order statistics of particle states that are ignored




**(a) Number density; t=0, t=0.7 s** **(b) Number density; t=0, t=1.0 s** **(c) Mean diameter; t=0, t=0.7 s**

**Fig. 3. PGM prediction of a polydisperse puff of water droplets in an ambient environment.**

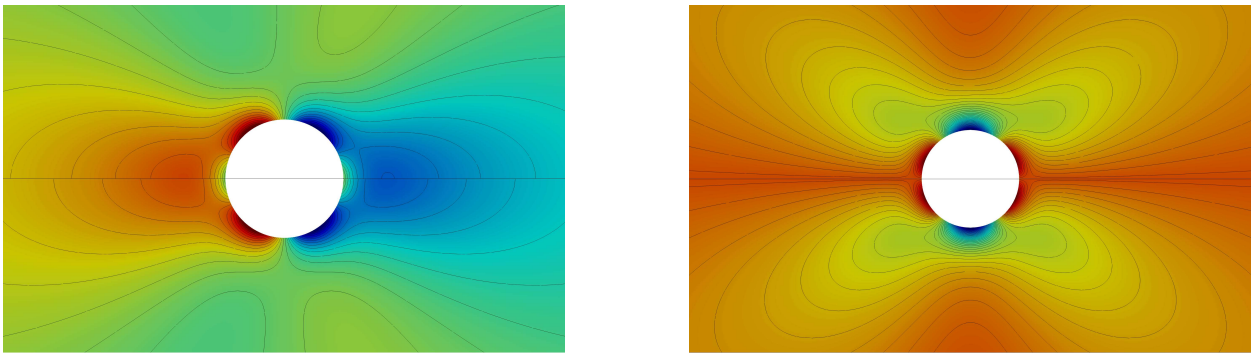
in many classical models opens the door for vastly improved accuracy of the predictions that are possible from computationally efficient Eulerian methods. Further refinement of the models will enable predictions of biological droplet dispersal that are much more accurate than those of traditional Eulerian methods.

## 2.2 Discretization Procedure

In addition to their physical modelling advantages, moment-based methods are highly desirable numerically, as they take the form of first-order hyperbolic balance laws. The first-order nature of the models has been shown to greatly increase the robustness of numerical solution of lower quality meshes [47], as compared to the numerical solution of the Navier-Stokes equations. These moment equations do, however, often have still local source terms. Fortunately, as the source terms are entirely local, they do not add global stiffness to the problem. Point-implicit time-marching methods can be used to efficiently advance numerical solutions.

In this work, the discontinuous-Galerkin-Hancock (DGH) method is selected. This numerical scheme was developed by Suzuki and van Leer specifically for the efficient and accurate solution of moment equations [22]. It is based on the upwind moment scheme of Huynh [48], and extends the method for the efficient solution of hyperbolic laws with stiff local sources. Somewhat remarkably, this coupled space-time method achieves third-order accuracy in both space and time, while only using linear elements [49, 50]. The DGH method can be implemented in a highly efficient manner for execution in parallel computational resources, as neighbouring cells only need to exchange information once per time step. Also, the time-step stability limit for the DGH method is far less restrictive that that of traditional high-order Runge-Kutta-DG methods, meaning larger time steps can safely be taken. The result is that the scheme can easily achieve extremely high parallel efficiency, even when hundreds of thousands of cores are used. It is also very amenable to implementation on unstructured grids or when adaptive mesh refinement (AMR) is used.

As a demonstration of the capabilities of the ten-moment model's ability to make predictions for traditional viscous flow problems and for the DGH scheme to compute high-accuracy solutions for moment equations, Figure 4 shows the classical situation of Stokes flow past a circular cylinder. The top half of each image shows the DGH numerical solution to the ten-moment equations, while the bottom half shows the exact solution to the Navier-Stokes equations. Figure 4(a) shows the deviatoric $x$-direction pressure, which is the negative of the traditional deviatoric fluid stress, $P_{xx} - p = -\tau_{xx}$. Figure 4(b) shows the shear pressure, which is the negative of the fluid shear stress, $P_{xy} = -\tau_{xy}$. Not only is it obvious that the first-order hyperbolic ten-moment equations are able to accurately predict viscous flow phenomena, but the high-accuracy of the DGH method is demonstrated, as this very low Mach number flow (Ma $\approx 0.0018$) is computed using a compressible solver without the need for low-Mach-number preconditioning.



**(a) The deviatoric $x$-direction pressure, $P_{xx} - p$.** **(b) The shear pressure, $P_{xy}$.**

**Fig. 4. DGH moment-method prediction (top half) and exact Navier-Stokes solution (bottom half) of Stokes flow past a circular cylinder.**

## 2.3 Project Milestones

**Milestone 1: Completion of the implementation, verification, and validation of the PGM model coupled with background flow.** Preliminary studies to date with the PGM model for aerosol dispersion have yet to include the effect of the turbulence in the background flow on the particle phase. To this end, a theoretical formulation has already been developed, the effect of which is to include an additional local source term in the model equations. Comparisons against predictions of stochastic modelling approaches for benchmark plume dispersion cases indicate a good agreement. In this milestone, we will focus on finishing the implementation, verification, and validation of the approach for cases relevant to airborne transmission. Thus, we would run lower-resolution benchmark case to evaluate the algorithm, make improvements to the physical model and the numerical approaches, and performance tune the application.

**Milestone 2: Completion of high-resolution computational studies of airborne transmission.** Full-scale computations of the dispersion of airborne polydisperse droplets will be undertaken. A variety of geometries and indoor conditions (humidity, temperature, airflow, air exchange rates, etc.) will be considered in order to construct a set of representative cases which will be used to fully validate the PGM as an efficient and accurate model for the prediction of bio-aerosol spread. Comparisons will be made with experiments that are currently underway at the Canadian Nuclear Laboratories and other available data in the literature.

**Milestone 3: Investigation of turbulent regimes in which non-continuum effects may manifest.** In this milestone, the full validation of the moment-closure approach for DNS of benchmark turbulent flows is undertaken by computing the ten-moment solution for the Taylor-Green vortex case on a $1,024^3$ grid. This will establish whether the ten-moment equations would fully agree with the traditional Navier-Stokes reference solution for this benchmark turbulent case, or not.

Following the validation of the ten-moment model's use for DNS computation of classical turbulence, we will target turbulent regimes for which the smallest scales are expected to be comparable to the molecular scales of the gas. It has long been estimated that, in some circumstances, the Kolmogorov scale of turbulence can approach the mean free path of a gas. Even when the regimes become close, traditional analysis estimates that viscous effects will damp turbulent eddies before non-continuum effects become significant. However, it is known that continuum models tend to over-estimate viscous effects at these scales. It is

therefore feasible that, in the right regimes, turbulence can be influenced by thermodynamic non-continuum phenomena. We will identify the regimes in which this is most likely to be the case and use the ten-moment model to compute DNS solutions. Results will be analyzed to verify if the fluid stresses deviate from those predicted by the Navier-Stokes equations. This can be done without a Navier-Stokes solution, as it only involves verifying if the fluid stresses are related to gradients of the velocity field in the traditional manner or not. This investigation will allow us to determine if the prevailing wisdom, that turbulence is *always* a continuum phenomenon, is true or not.

## 3 COMPUTATIONAL READINESS

### 3.1 Use of Resources Requested

The resources required for **Milestone 1** are estimated according to our previous effort to implement and verify the PGM, ten-moment model, and DGH approaches using a DD allocation. For this effort, we have used about 50,000 node-hours, and we anticipate to require a similar level of effort for the development work outlined in this milestone, which includes performing lower-resolution simulations, improvements to the physical model and numerical approaches, and performance tuning. We anticipate this effort to mostly occur within the first three to four months of the project, and to require periods of peak usage.

For the purpose of estimating the allocation requirements for **Milestone 2**, we have considered a reference case which consists in simulating the unsteady dispersion of a pathogen-laden particle phase following a violent respiratory event in a typical indoor environment (e.g., standard room) for four seconds of real time. Preliminary, unoptimized, simulations performed on Theta KNL with 1st-order discontinuous-Galerkin method show that a minimum allocation on ALCF Theta KNL of 128 nodes (or 8,192 KNL cores) allows to perform the reference simulation using a computational grid with approximately 4.2 million elements in about two hours. The planned production runs will use the third-order DGH scheme that has vastly improved accuracy at an additional computational cost of roughly an order of magnitude. Note that simulations of larger domains or longer times will require about five to ten times more resources. Additionally, we are considering the application of our AMR approach, which would be critical to tracking relevant spatial scales more efficiently, especially in the presence of multiple sources of contamination, which would in turn provide at least another order of magnitude reduction in the computational cost of the production level runs. Our goal is to track the aerosol dispersion accurately on spacial and temporal scales relevant to establishing the contamination risk for the particular conditions of the problem (e.g., minutes to tens of minutes). Therefore, we expect that an average run would require about 5,000 node-hours. We consider 20 production runs which would lead to 100,000 (20 x 5,000) node-hours for production-type simulations, for a total of 150,000 node-hours dedicated to the first scientific goal (see Sect. 1.1). The simulations are expected to be spread out uniformly throughout the lifetime of the allocation.

Furthermore, we estimate to use 850,000 node-hours for performing DNS investigations of turbulent flows with moment-closure models, which is the second scientific goal of the proposal (see Sect. 1.2). For **Milestone 3**, we will further carry out detail simulations of the Taylor-Green vortex problem. Our estimate is based on preliminary investigations with DGH method and the ten-moment model on ALCF Theta KNL for a mesh of $512^3$ elements (i.e., approximately 134 million elements). For a fully-resolved calculation we estimate to require meshes on the order of $1,024^3$ elements (approximately 1,073 billion elements). Based on our previous computations we estimate that we can run three to four fully resolved calculations with 850,000 node-hours. This will allow us to study a range of conditions for regimes in which non-continuum effects are most likely, thereby demonstrating the feasibility of the proposed idea. We anticipate to require only minor performance tuning for running these cases and therefore, the simulations are anticipated to

occur soon after the allocation is granted.

Output and restart files for the aforementioned runs are on the order of terabytes, and our total request is up to 30 TB. Part of the data will be transferred to local machines where appropriate using ssh and/or Globus services. For the processing of large data sets, we will use *in-situ* analysis and/or remote visualization techniques.

## 3.2 Computational Approach

The application software, `BLawB`, represents the main code to be used for carrying out the proposed research. `BLawB` (Balance Law Bargain) is an in-house code under development in Prof. J. G. M$^{c}$Donald's research group at the University of Ottawa and Dr. L. Ivan's research team at Canadian Nuclear Laboratories. The `BLawB` computational framework has been designed for performing massively-parallel simulations on distributed and shared-memory (CPU) architectures. The code solves various balance-law equations, mostly for the transport phenomena occurring in multiphase flow problems. A dimensionally-agnostic discontinuous-Galerkin-Hancock formulation on general elements (e.g., triangular, quadrilateral, tetrahedral, hexahedral) of third-order coupled space-time is used in conjunction with mesh adaption for the solution of hyperbolic-relaxation PDEs describing moment-closure models. In particular, a recently proposed polydisperse Gaussian-moment model (PGM) is used to simulate particle-laden flows within an Eulerian formulation that directly treats high-order particle statistics that are neglected in traditional models such as the variances and covariances between particle velocities, sizes, and any other properties of relevance.

`BLawB` uses multi-block structured and unstructured grid approaches. The large-scale domain decomposition of the grid is performed via block-based adaptive mesh refinement. The DGH formulation has a high local work to communication ratio, thereby it is highly amenable for parallelization on a massive scale. Parallelization of the code is achieved with MPI and OpenMP libraries with most parallelization tasks being generated at the block level. The code has been routinely run on ALCF Theta KNL and SciNet Niagara (Compute Canada centre) machines, and has been shown in numerical experiments to have extremely efficient scalability up to hundreds of thousands of CPU cores. Figure 5 demonstrates the strong scalability of the code for the Taylor-Green problem described above.

The software, `BLawB`, depends on several standard external libraries, all of which are available freely under permissive open-source licenses. The required external libraries are included in Table 1.

**Table 1. Required external libraries**

| Library | Use | License |
|---|---|---|
| VTK | Visualization and data-file production | BSD |
| Eigen3 | Linear algebra | MPL2 |
| Chaiscript | Input parsing and problem initialization | BSD |
| Pybind11 | Input parsing and problem initialization | BSD |
| Cereal | Data serialization | BSD |
| Boost C++ | Automatic differentiation and serialization | Boost Software License |

The `BLawB` software has already been deployed on Theta KNL and these libraries exist or have been already locally installed on the system. The restart capability has been tested and used on the system.

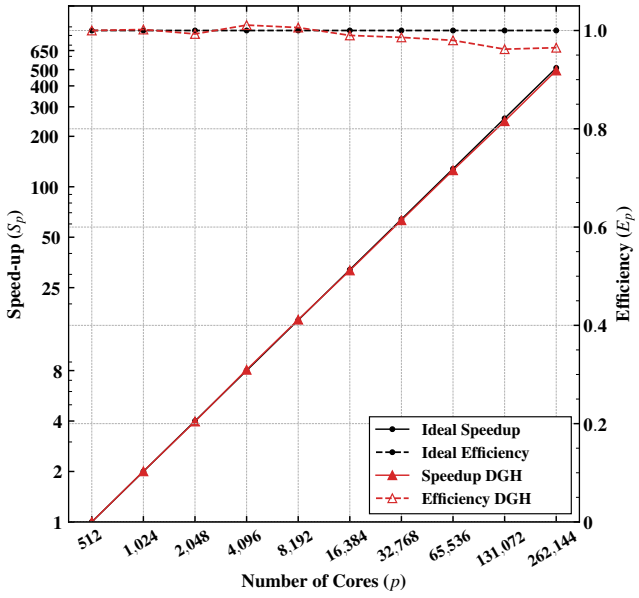



**Fig. 5. Strong scaling analysis for the Taylor-Green vortex problem.**

### 3.3 Developmental Work

The `BLawB` software has already been built and used on ALCF Theta KNL. Though we continue to profile and improve the efficiency of the code, the majority of the needed implementation is running and verified. Remaining implementation work includes the local source terms in the PGM for evaporation modelling, as well as considering the effect of turbulent background flow on the particle phase, for which a theoretical formulation has already been derived. Both of these additions will be verified before moving on to production runs. The evaporation model can easily be compared to available exact solutions for simple problems, while the interaction between background turbulence and the particle phase will be compared to benchmark plume models. These developments are currently underway under our DD allocation, and it is possible they will be completed before this proposed allocation would begin.

**Proposal Title:** Novel high-fidelity moment closures for polydisperse multiphase and turbulent flows

| **Milestone:** | **Details (as appropriate):** | **Dates:** |
|---|---|---|
| 1. Completion of the implementation, verification, and validation of the PGM model coupled with background flow | **Resource:** Theta KNL **Node-hours:** 50,000<br>**Filesystem storage (TB and dates):** 1 TB (January 2023 - April 2023)<br>**Archival storage (TB and dates):** 0 TB<br>**Software Application:** `BLawB`<br>**Tasks:** lower-resolution simulations, improvements to the physical model and numerical approaches, performance tuning<br>**Dependencies:** None | January 2023 - April 2023 |
| 2. Completion of high-resolution computational studies of airborne transmission | **Resource:** Theta KNL **Node-hours:** 100,000<br>**Filesystem storage (TB and dates):** 4 TB (June 2023 - December 2023)<br>**Archival storage (TB and dates):** 0 TB<br>**Software Application:** `BLawB`<br>**Tasks:** run production-type case, analyze data<br>**Dependencies:** Milestone 1 | June 2023 - December 2023 |
| 3. Investigation of turbulent regimes in which non-continuum effects may manifest | **Resource:** Theta KNL **Node-hours:** 850,000<br>**Filesystem storage (TB and dates):** 25 TB (Jan 2023 - December 2023)<br>**Archival storage (TB and dates):** 0 TB<br>**Software Application:** `BLawB`<br>**Tasks:** perform the target DNS runs with moment-closure approach<br>**Dependencies:** None | January 2023 - December 2023 |

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## PERSONNEL JUSTIFICATION AND MANAGEMENT PLAN

### PERSONNEL JUSTIFICATION

All personnel included below is already in place and got accounts on ALCF Theta KNL system.

| Name | Title | Affiliation | Project Role |
|---|---|---|---|
| Dr. L. Ivan | Computational Research Scientist | CNL* | PI, developer, analysis |
| Prof. J.G. M$^{c}$Donald | Associate Professor | UOttawa** | Co-PI, developer, analysis |
| W. Kauffmann | PhD Student | UOttawa** | developer, simulations, analysis |
| O. El-Ghotmi | Master's Student | UOttawa** | developer, simulations, analysis |
| B. Allard | Master's Student | UOttawa** | developer, simulation, analysis |
| F. Forgues | Computational Research Scientist | CNL* | simulations, analysis |

* Canadian Nuclear Laboratories, 286 Plant Road, Chalk River, Ontario, Canada K0J 1J0
** Department of Mechanical Engineering, University of Ottawa, Ottawa, Ontario, Canada K1N 6N5

### MANAGEMENT PLAN

Dr. Ivan and Prof. M$^{c}$Donald represent the project's leadership team, and will decide how the compute time is allocated to each individual team member such that the goals and millstones of the project are achieved.

Dr. Ivan will act as the point of contact to provide updates on the status of the work including publications, awards, and highlights of accomplishments.

All six team members will have weekly meetings to discuss the progress of all aspects of the project. The PI and Co-PI will be involved at every level of the project and provide supervision to junior staff and students, who will perform the bulk of the simulation runs and direct post-processing of the data. The PI and Co-PI will also carry out code development and interpretation of the results. Kauffmann will be responsible for numerics and turbulence studies, with support from El-Ghotmi. Allard and Forgues will perform verification, validation, and production-level simulations of multiphase flows for the airborne trasmission cases considered.

# Dr. Lucian IVAN

**Computational Research Scientist**
**Advanced Reactor Directorate, Canadian Nuclear Laboratories (CNL)**
**286 Plant Road, Chalk River, Ontario, Canada K0J 1J0**
**Work:+1 613 584 3311 ext. 42592, lucian.ivan@cnl.ca**


## Professional Preparation

| | |
|---|---|
| PhD | Aerospace Engineering, University of Toronto, Toronto, Canada, 2010 |
| MS | Aerospace Engineering, Politehnica University of Bucharest, Romania, 2000 |
| BS | Aerospace Engineering, Politehnica University of Bucharest, Romania, 1998 |

## Appointments

| | |
|---|---|
| 2015–present | Computational Research Scientist, Canadian Nuclear Laboratories, Canada |
| 2020–present | Part-time Professor, Department of Mechanical Engineering, Univ. of Ottawa, Canada |
| 2014–2015 | Research Associate, Department of Applied Mathematics, Univ. of Waterloo, Canada |
| 2010–2014 | Postdoctoral Fellow, Department of Applied Mathematics, Univ. of Waterloo, Canada |
| 2009–2010 | Research Assistant, Department of Applied Mathematics, Univ. of Waterloo, Canada |
| 2002–2010 | Doctoral Candidate, Aerospace Engineering, Univ. of Toronto, Canada |
| 1999–2002 | Design Engineer, Turbomecanica SA, Romania |
| 1998–1999 | Design Engineer, National R&D Institute for Gas Turbines COMOTI, Romania |

## Five Publications Most Relevant to This Proposal


1. M. Marchildon, B. Allard, L. Ivan, J. G. M$^{c}$Donald, ‘‘A Surface-Weighted Polydisperse Gaussian-Moment Method for Modelling Atmospheric Dispersion of Evaporating Particles, to be submitted to J. Computational Physics, 2022

2. R. Taylor, C.P.T. Groth, Z. Liang and L. Ivan, ‘‘Mesh-Independent Large-Eddy Simulation with Anisotropic Adaptive Mesh Refinement for Hydrogen Deflagration Prediction in Closed Vessels”, In Proceedings of the 8th International Conference on Hydrogen Safety, Australia, 2019.

3. F. Forgues, L. Ivan, A. Trottier and J. G. M$^{c}$Donald, ‘‘A Gaussian Moment Method for Polydisperse Multiphase Flow Modelling”, J. Computational Physics, Vol. 398, 108839, 2019

4. L. Freret, L. Ivan, H. De Sterck and C.P.T. Groth, ‘‘High-Order Finite-Volume Method with Block-Based AMR for Magnetohydrodynamics Flows”, J. Scientific Computing, Vol. 79, pp. 176-208, 2019

5. D. Hummel and L. Ivan, ‘‘Near-field investigation of the explosive dispersal of radioactive material based on a reconstructed spherical blast-wave flow”, J. Environmental Radioactivity, Vol. 172, pp. 30-42, 2017


## Research Interests and Expertise

Dr. Ivan has solid expertise in the development of scalable, high-performance computing algorithms on modern architectures, which include high-order schemes and adaptive mesh refinement approaches, for the simulation of fluid, plasma, multiphase and particle-laden flows under a range of conditions. His work has focused on modeling and simulation of physically complex flows characterized by disparate temporal and spatial scales such as those encountered in atmospheric dispersion and deposition of plume and aerosol, large-eddy simulation of turbulent combusting flows in large-scale vessels, and computational space-plasma physics. His research interests include moment closure methods, data assimilation algorithms and inverse problems, radiation transport methods, modelling of transport processes in the human eye structures, and quantum computing. He is also active in the additive manufacturing nuclear community as a representative of Canada and CNL in the Generation IV International Forum (GIF) Advanced Manufacturing and Material Engineering Task Force (AMME TF).

**Synergistic Activities**

1. **Co-organizer of the "AMME Virtual Workshop on Advanced Manufacturing" Workshop, Virtual, Canada, 2021.**

   As a a representative of Canada and CNL in the GIF AMME TF, I have co-organized this international workshop focused on how Modelling and Simulation (M&S) can be used to enable the qualification of advanced manufactured components in the nuclear field. The workshop has brought together representatives from 16 nuclear energy-producing countries active in academia, industry, and regulatory bodies.

2. **Co-organizer of the "Society of Canada Computational Fluid Dynamics (CFD)" Conference, University of Waterloo, Waterloo, Canada, 2015.**

   The CFD Society of Canada has been holding its annual conference since 1993. This international conference brings together experts from academia, industry and government to discuss current and future issues in the development and application of CFD.

3. **Participant in High-Performance Computing Training**

   I was part of the 2014 Argonne Training Program on Extreme-Scale Computing (ATPESC) which provides intensive, two weeks of training on the key skills, approaches, and tools to design, implement, and execute computational science and engineering applications on current high-end computing systems and the leadership-class computing systems of the future. Additionally, I frequently attend workshops and/or webinars in high-performance computing organized by ALCF (e.g., Aurora Learning Path) or Exascale Computing Project (ECP).

4. **Teaching of High-Performance Computing Courses**

   Since 2020, I have been a Part-time Professor in the Department of Mechanical Engineering at the University of Ottawa where I have taught graduate-level courses in high-performance computing.

5. **Graduate Student Supervision**

   I have provided supervision to seven internship graduate students from diverse fields (e.g., quantum computing, combustion modelling, two-phase flows for thermohydraulics, polydisperse multiphase flow modelling) at the Canadian Nuclear Laboratories (CNL). I am also regularily co-advising graduate students in the Department of Mechanical Engineering at the University of Ottawa and the Institute for Aerospace Studies at the University of Toronto.

**Collaborators (*past 5 years including name and current institution*)**

**Prof. James G. McDonald**, Department of Mechanical Engineering, Univ. of Ottawa, Canada
**Prof. Clinton P.T. Groth**, Univ. of Toronto Institute for Aerospace Studies, Canada
**Prof. Hans De Sterck**, Department of Applied Mathematics, Univ. of Waterloo, Canada
**Dr. Zhe Liang**, Canadian Nuclear Laboratories, Canada
**Dr. Luke Label**, Canadian Nuclear Laboratories, Canada
**Dr. Alexandre Trottier**, Canadian Nuclear Laboratories, Canada
**Dr. Isabella J. van Rooyen**, Pacific Northwest National Laboratory, USA
**Dr. Mark Christian Messner**, Argonne National Laboratory, USA
**Dr. Lucie Fréret**, Maya HTT, Canada
**Prof. Lyndon Edwards**, Australian Nuclear Science & Technology Organisation, Australia

**Dr. James MCDONALD**
**Associate Professor**
**Department of Mechanical Engineering**
**University of Ottawa**
**161 Louis Pasteur, Ottawa, Ontario, Canada, K1N 6N5**
**Work:+1 613 562 5800 ext. 6249, James.McDonald@uOttawa.ca**

**Professional Preparation**

| | |
|---|---|
| PhD | Aerospace Engineering, University of Toronto, Toronto, Canada, 2011 |
| MASc | Aerospace Engineering, University of Toronto, Toronto, Canada, 2005 |
| BEng | Mechanical Engineering, Dalhousie University, Halifax, Canada, 2003 |
| BA | Music, Dalhousie University, Halifax, Canada, 2003 |

**Appointments**

| | |
|---|---|
| 2020–Present | Associate Professor, University of Ottawa, Ottawa, Canada |
| 2013–2020 | Assistant Professor, University of Ottawa, Ottawa, Canada |
| 2010–2013 | Post-Doctoral Fellow, Rheinisch-Westfälische Technische Hochschule (RWTH University), Aachen, Germany |
| 2003–2010 | Master's and Doctoral Student, University of Toronto, Toronto, Canada |

**Five Publications Most Relevant to This Proposal**

1. M. Marchildon, B. Allard, L. Ivan, J. G. M$^{c}$Donald, ''A Surface-Weighted Polydisperse Gaussian-Moment Method for Modelling Atmospheric Dispersion of Evaporating Particles", to be submitted to Journal of Computational Physics, March 2022
2. F. Forgues, L. Ivan, A. Trottier and J. G. M$^{c}$Donald, ''A Gaussian Moment Method for Polydisperse Multiphase Flow Modelling", Journal of Computational Physics, Vol. 398, 108839, 2019
3. C. Yan and J. G. M$^{c}$Donald, ''Hyperbolic Turbulence Models for Moment Closures", Journal of Computational Physics, Vol. 422, 109753, 2020
4. F. Forgues, and J. G. M$^{c}$Donald, ''Higher-Order Moment Models for Multiphase Flows With Accurate Particle-Stream Crossing", International Journal of Multiphase Flow, Vol. 114, pp. 28–38, 2019
5. S. Boccelli, F. Giroux, T. E. Magin, C.P.T. Groth, and J. G. M$^{c}$Donald, ''A 14-Moment Maximum-Entropy Description of Electrons in Crossed Electric and Magnetic Fields", Physics of Plasmas, Vol. 27, 123506, 2020

**Research Interests and Expertise**

Professor McDonald is a pioneering researcher in the field of hyperbolic maximum-entropy moment methods. These methods, derived from the kinetic theory of gases, offer the promise of many advantages as compared to traditional fluid-mechanics models, such as the Navier-Stokes equations. From a physical accuracy perspective, these moment models offer an expanded range of physical validity, as they are not derived based on a continuum assumption and can thus remain valid for flows that are out of local thermodynamic equilibrium. The hyperbolic nature of the results laws also predict finite speeds of information propagation, which is in contrast with the Navier-Stokes equations which allow for infinite speeds of information travel. From a numerical perspective, the first-order balance-law form of the governing partial differential equations give moment methods computational advantages. Often an extra order

of spacial accuracy can be achieved for a given numerical stencil, and numerical solutions have been shown to be far less sensitive to low quality meshes that are typical of practical geometries.

Professor McDonald's original work on maximum-entropy moment methods was applied to rarefied and micron-scale gas flows. More recently, he has adapted his techniques in order to develop new models for polydisperse multiphase flows, radiation modelling, classical and relativistic plasma flows, as well as quantum mechanics through the development of moment-based approximations to the Wigner equation.

In addition to his modelling work, Professor McDonald is also an expert on high-order numerical methods and large-scale scientific computing. He is the original author of the `BLawB` computational framework for the accurate and efficient solution of hyperbolic balance laws. This code is based on the discontinuous-Galerkin-Hancock method and is third-order accurate in space and time. It has been shown to scale to hundreds of thousands of computational cores with near perfect efficiency.

**Synergistic Activities**

1. **Member of Expert Review Committee, Compute Canada, 2014-2021**

   Reviewed and ranked applications for access to Canada's academic super-computer facilities.

2. **Co-organizer of the "Workshop for Moment Methods in Kinetic Theory II", Fields Institute for Research in Mathematical Sciences, Toronto, Canada, 2014.**

   This workshop brought together the world-leading experts in the field of moment methods for gas dynamics, radiation modelling, and multiphase flow prediction. It was funded by grants from the Fields Institute, the National Science Foundation, University of Toronto, and the University of Ottawa.

3. **Invited Presentations**

   I am regularly invited to give invited talks regarding my work on moment methods at international workshops and conferences as an invited speaker. Since 2013, I have given 13 invited talks on the subject. This is in addition to my regular presentations at national and international scientific conferences.

4. **Scientific-Computing Curriculum Development**

   I am a member of the Curriculum Committee in the Mechanical Engineering department at the University of Ottawa, where I am working to integrate scientific computing into the undergraduate curriculum in a holistic way. I have also created and integrated three new scientific computing and numerical methods courses to the curriculum, one at the undergraduate and two at the graduate level.

5. **Research-Opportunity Outreach to Undergraduate Students**

   I am a firm believer that undergraduate engineering students should be exposed to real research. At the University of Ottawa, students have the option of replacing two fourth-year electives with a research thesis. Since 2014, I have volunteered to supervise 27 undergraduate theses and research projects. This is in addition to the 26 graduate students I have supervised in that time.

**Collaborators (*past 5 years including name and current institution*)**

**Dr. Lucian Ivan**, Canadian Nuclear Laboratories, Canada
**Prof. Thierry Magin**, von Kármán Institute for Fluid Dynamics (VKI), Brussels, Belgium
**Prof. Clinton P.T. Groth**, University of Toronto Institute for Aerospace Studies, Toronto, Canada
**Prof. Matei Radulescu**, University of Ottawa, Ottawa, Canada
**Dr. Alexandre Trottier**, Canadian Nuclear Laboratories, Canada

# 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**

BLawB

**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.**

Directly from ALCF staff.

**Question #2**

**Suggested Reviewers**

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

Rodney Fox, Iowa 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.*

*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.*

**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.**

NoFile.pdf
The attachment is on the following page.

We do not require testbed resources at the present time.