2023 INCITE Proposal Submission
Proposal

Title: Cavitation inception in turbulent liquid metal
Principal Investigator: Mark Kostuk
Organization: General Atomics
Date/Time Generated: 6/15/2022 4:25:46 PM

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.*

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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

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Institutional Contact Phone

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Institutional Contact Email

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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 first ever high resolution compressible fluid simulations of the liquid mercury pressure wave created within the Spallation Neutron Source User Facility (SNS) will improve our understanding of the physics used to design and extend the lifetime of its target device. The SNS supports hundreds of researchers investigating a wide range of questions in fundamental science.

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.*

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

Node Hours

812000

Storage (TB)

31

Off-Line Storage (TB)

31

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

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

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.**

INCITE_ALMA_SNS.pdf
The attachment is on the following page.

PROJECT EXECUTIVE SUMMARY

Title: Cavitation inception in turbulent liquid metal

PI and Co-PI(s): M. Kostuk[1] (PI), E. Dominguez-Ontiveros[2], J. Weinmeister[2], A. Deshpande[1]

Applying Institution/Organization: 1. General Atomics, 3550 General Atomics Ct. San Diego, CA 92121
2. Oak Ridge National Laboratory, P.O. Box 2008 Oak Ridge, TN 37831

Resource Name(s) and Number of Node Hours Requested: 812k Summit node-hours

Amount of Storage Requested: 31 TB

Executive Summary:

The Spallation Neutron Source (SNS) is a Department of Energy (DOE) Office of Basic Energy Sciences (BES) user facility that impacts a proton beam of 1.4 MW into a turbulent liquid mercury target, generating neutrons that are used for scattering and imaging research. This facility enables over 350 publications each year in a wide range of fundamental sciences.

Imparting such high power into the mercury creates rapid heating, on the order of 10^7 K/s, resulting in sudden volumetric expansion and strong pressure waves within the target. These pressure waves interact with the turbulent shear flow of the mercury as well as the solid walls of the target, which deforms as it absorbs the pressure energy. The regions of extreme pressure drop that result within the mercury leads to cavitation (on a sub-millimeter scale), eroding the walls of the target vessel. Understanding this pressure wave, and the mechanisms of cavitation inception within turbulent liquid metal, ultimately improves the target design and lifetime within its harsh operating environment. Pursuing this understanding can have a compounding impact on fundamental science research in the United States during the remaining decades of SNS operation.

In this project, the first ever high resolution simulations of this pressure wave propagating through a turbulent liquid metal will be performed. A high fidelity representation of mercury's equation of state and temperature dependent viscosity will be used, along with an accurate target geometry and an experimentally accurate heat deposition profile, to capture the 23 kJ that are deposited within 0.7 μs.

The simulations will be carried out by the compressible, finite-difference flow solver developed by General Atomics called ALMA, that has demonstrated running at large scale on Summit. ALMA is fully GPU-accelerated and implements an antisymmetric representation of the fluid equations and time evolution operator, such that conserved quantities (e.g. mass, momentum and energy) are preserved regardless of the grid or chosen numerical scheme. The resultant numerical stability is essential when computing over the 13 B fluid elements required for this multiscale phenomenon.

The requested simulations total 812k Summit-node hours of capability computing (44% of Summit) to model the energy deposition and resulting pressure waves at a high fidelity to understand the expected pressure distributions in the target before solid wall deformation. This data is the foundation for a study of multiple beam powers to understand the effect of operating conditions on cavitation inception, an investigation of sequential beam pulses (it operates at 60 Hz), and will inform future modeling efforts.

The collaborative team from General Atomics and Oak Ridge National Laboratory include both subject matter experts on the SNS, and co-authors of the ALMA fluid solver, working together on this transformative project of the multiphysics engineering challenge presented by the SNS, as understanding pressure propagation through a fluid has been impossible to date.

Cavitation inception in turbulent liquid metal

1 Significance of Research

The Spallation Neutron Source (SNS) is a Department of Energy (DOE) Office Science user facility utilized primarily for neutron scattering research [1]. The SNS is a pulsed neutron source facility which uses a linear particle accelerator to produce a proton beam which impacts a liquid mercury target to create neutrons via a spallation process. These neutrons are utilized for a variety of fundamental materials research. The reliable, high-performance operation of the SNS target is critical to ensure the high throughput of fundamental research that the SNS enables as a user facility for the DOE Office of Science. However, analysis of the target is complicated by the intense multiphysics environment in which it operates.

While the SNS is primarily a neutron scattering facility, some neutron imaging and neutron physics instruments exist. The SNS instruments enable approximately 350 publications a year in fundamental engineering, biological, and quantum materials alongside research in soft matter, chemistry, and high-pressure science. Critical to these research outcomes is a high quality neutron source, which can be measured in both the intensity of the neutron beam (facility power) and amount of run time. As an overview, the SNS facility is composed of a linear particle accelerator, accumulating ring, target, and instruments. To start, a hydrogen atom is doped with an additional electron and injected into the start of the linear accelerator where obtains an energy of 1 GeV before a diamond foil strips the electrons from the proton. Then, proton bunches are formed in the accumulator ring before being injected into the target at a frequency of 60 Hz. The target is flowing liquid mercury housed in a 316L stainless steel vessel. The protons impact the mercury, and via a spallation process, produce an abundance of neutrons. Some of these neutrons then move through moderators which thermalize them before they proceed down beam tubes to individual instruments arranged around the target. The neutrons then interact with samples and are detected within each instrument. Data reduction is then performed on this raw data to extract research results [2].

While the SNS was commissioned in 2008, it has undergone improvements throughout its lifetime which have improved the utility of the facility. Among these improvements are changes to the SNS target. Over the operating life of the SNS, multiple target failures, due to both weld failures and cavitation erosion, have imperiled neutron production. As such, the facility has not always been able to operate at maximum power and has also had to change its target replacement schedule [3]. The SNS currently operates at 1.4 MW with an impending upgrade project to increase the total power to 2 MW with proton energies of 1.3 GeV. These improvements will provide scientists with an increased ability to probe materials and conduct research. An Additional limitation is the total available beam time. If targets can be designed to last longer with less time between planned outages i.e., if the facility can be designed to operate for longer run cycles at higher powers, it will be able to provide greater impetus to the ongoing SNS-enabled research. However, this goal is impeded by the difficulty in designing and qualifying such a high performance target. Regardless, these target improvements are worth pursuing due to the potential impact over the projected remaining decades of operating life alongside pressure from competing neutron sources around the world.

Fundamentally, improving the target design requires understanding the complex multiphysics environment in which it operates. This environment requires modeling the proton beam, neutron transport, nuclear heating, fluid flow, and solid mechanics. Most important to the target is accurate modeling of the coupled, complex physics of the target fluid (mercury) and solid vessel (stainless steel). The energy deposition in the target is extreme, with each proton pulse delivering 23 kJ in only 700 ns, though it can be modeled at the needed fidelity using a radiation transport code like MCNPX [4]. This energy deposition creates abrupt heating in the mercury, on the order of 10^7 K/s, resulting in rapid volumetric expansion and strong pressure waves within the target [5]. These pressure waves interact with the turbulent flow within the target as well as the solid walls of the target, which deforms as it absorbs the pressure energy. These deformations and pressure waves create tension forces within the mercury, resulting in cavitation which erodes the walls of the target vessel. It is believed that the cavitation inception occurs at sub-millimeter and even micron scale within the fluid. Finally, the SNS target has recently been modified for helium gas injection to mitigate the pressure waves within the target. This gas injection reduces both measured strains on the target vessel [6] and the amount of measured cavitation erosion [7]. As such, all of the above physics must be understood and accounted for in the design of the mercury target to determine its operating lifetime.

The facilities required to physically study a target under energy deposition are prohibitively expensive, so computational studies are required for target analysis. However, the coupled multiphysics of the target make computational studies difficult to perform reliably and at the necessary fidelity. A computational fluid dynamics (CFD) solver is required which can simultaneously solve two-phase turbulent flow alongside cavitation and fluid-structure interaction at a superfine (DNS-level) resolution, which is currently not feasible for moderate to high-Reynolds number flows. Some current commercial CFD solvers have the capability to solve all of the required physics, with unknown reliability, though they can not run on a the GPU-accelerated leadership class computers which are required for the fine resolution required for accurate modeling. This work seeks to better understand part of the physical process by accurately modeling the energy deposition and resulting pressure waves at a high fidelity to understand the expected pressure distributions in the target before gas injection and solid wall deformation. This ability is transformative for the multiphysics engineering challenge as understanding this pressure wave creation and propagation through turbulent liquid mercury has been impossible to date.

An artistic rendering of the SNS target is shown in Fig. 1 with a detail of previously seen cavitation erosion. The target is cantilevered away from its carriage assembly to allow the neutron moderators to sit directly above and below it. The target vessel is composed of two walls of 316L stainless steel with mercury flowing within and a vacuum outside. The total mercury flow is approximately 250 GPM with the majority flowing through two bulk inlets on either side. In addition, a small amount of flow (~ 25 GPM) flows through the window channel between the two vessel walls and through jet flow ribs which sweep up the main target window which the proton beam enters through. All flow exits a central outlet. The vessel has several rib structures within to separate these flow regions. The flow is highly turbulent with a characteristic Reynolds number of approximately 7.1×10^5 and curved surfaces which make the flow turbulence anisotropic in regions. Further, the bulk flow layout induces a stagnation region near the proton window and periodic vortices in recirculation regions attached to the flow-dividing ribs.

Previous research has investigated the SNS target using a variety of tools which only partially cover the entire set of phenomena that govern its performance. Finite element analysis (FEA) of the mercury

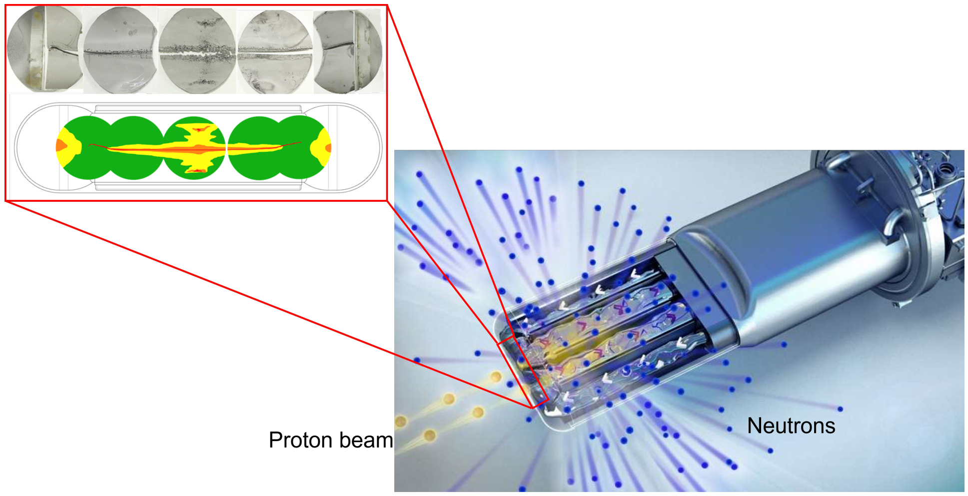

Figure 1: An artistic rendering of the SNS target showing the mercury flow path, neutron production, and an example of cavitation erosion. The mercury flows in from the outer channels (white arrows) and returns in the center (purple arrows). The incident proton beam (yellow) hits the front center of the target and produces neutrons (blue) which travel in all directions. The example cavitation erosion is shown on disks cut from a target's inner window after operation, with the disk locations shown in the color plot below them. Note that the cavitation was severe enough to initiate a crack along the entire width of the window.

target has been an especially fruitful area of research for the SNS target under its historical operating regime. FEA was first validated for the mercury and vessel under power deposition using the ABAQUS code for both a cylindrical and prototypical shape against data collected at the Los Alamos Neutron Science Center - Weapons Neutron Research (LANSCE-WNR) facility [8]. This model predicts the dynamic strain response of the target by modeling the mercury as a solid with a custom Equation of State (EOS) model. For the work, a Mie-Gruneisen model is utilized with a tensile cutoff pressure of 0.15 MPa to simulate the onset of cavitation within the mercury. This model was able to correlate areas which experienced a long time under tension with areas of high cavitation erosion in the target [4]. This model has also been extended for simulations with mercury gas injection by using proportional, integral, and derivative (PID) control [9] and optimized using Bayesian calibration [10]. However, these interpolative tools are of limited value for future designs and operations which fall outside the existing strain validation data sets. This is especially true when considering the complex flow patterns and multi-phase state of new target designs for 2 MW operation.

Flow effects have been studied as well, though they have been limited by computational and experimental limitations. Computationally, CFD studies have been limited to incompressible Reynolds-Averaged Navier-Stokes (RANS) computations of the SNS target [11–18] and focused on bulk flow behavior and vessel temperature prediction. The one exception is the work of Wendel, Geoghegan, and Felde [16], which looked at creating higher shear flow along the target inner window to prevent cavitation erosion by re-directing impinging jets. All of these simulations, though, used a relatively coarse grid with a two-equation turbulence closure based on Boussinesq's eddy viscosity assumption. Additionally, these works modeled power deposition as a steady-state phenomena by time-averaging the individual pulses, so no transient effects have been modeled to date. In reality, transient and non-isotropic turbulence are important to the target's performance. Turbulence in the flow interacts with the pressure waves distorting it to create asymmetries and quasi-periodic flow instabilities which are difficult to capture in RANS calculations [14]. Previous studies [19–21] have established relationship between cavitation inception and quasi-streamwise vortices in a turbulent shear layer generated by flow separation. Since localized regions of separation are also observed in this case, we may expect a similar phenomenon to occur. Therefore, resolution of turbulent structures is necessary to investigate this hypothesis. Liquid mercury also acts as a coolant for the SNS target, in addition to serving as the neutronic target medium. Therefore resolving near-wall turbulence is essential in getting accurate estimates of heat transfer at the surface by accounting for localized phenomena such as viscous dissipation at Kolmogorov length scales and turbulent transport of heat.

This work aims to address these issues by using the Anti-symmetric, Large-Moment, Accelerated fluid solver (ALMA) [22] for carrying out highly resolved Implicit Large-Eddy Simulations (ILES). To the best of our knowledge, this is a first of a kind study that aims to calculate a time-accurate flowfield that will potentially aid in more effective design of the SNS target to increase the longevity of its operation. Some of the challenges involved in performing fluid simulations of the target (which are more relevant to this proposal) are listed below;

1. The high Reynolds number of the flow in consideration ($Re \approx 7.1 \times 10^5$) demands sufficient near-wall resolution for an ILES run, wherein the inherent numerical dissipation acts as a sub-grid scale model. This eventually translates to a large problem size $\left(\sim \mathcal{O}\left[10^{10}\right]\right)$ points [23], that require state-of-the-art petascale and exascale resources.
2. Studying cavitation in this scenario requires resolving a broad range of pressure values, ranging from a few Pascals to mega-Pascals. This results in a stiff system and can potentially cause numerical instability.
3. Behaviour of liquid mercury deviates significantly from the Mie-Gruneisen model. Hence more sophisticated equations of state are required to establish relationship between thermodynamic state variables. These are only valid for a limited range of pressure and density and therefore reconciling different equations that model the bulk flow and cavitation concurrently is not trivial.

Previous experimental studies of the target have produced a plethora of useful data, though the cost of studies using proton bombardment coupled with instrumentation challenges prohibit detailed studies of the problem subject to all the physical phenomena. However, these studies have produced useful and extensive validation data sets which ensure the reliability of computational models. This data includes particle image velocimetry (PIV) data for a water flow field in the target geometry [17, 18] which can be utilized to validate the overall flow field of a target simulated using CFD. Additionally, this data includes strain and pressure distribution for basic and prototypical geometries [8] alongside the actual target [6, 24, 25] for both pure mercury and helium gas injection operation. This data provides an excellent validation dataset for peak pressure and vessel strain prediction. Finally, post irradiation examination efforts have produced data on the location and extent of cavitation erosion on the vessel wall [26] which can be used to validate cavitation prediction [4] despite the erosion not being physically modeled.

This research will fill a need in multiphysics simulation capability that can not be filled by existing simulation capabilities. While transient pressure data can be extracted from simulations where mercury is modeled statically, known effects from the mercury flow field prevent these tools from reaching high accuracy in predictive scenarios. This is compounded when two-phase flow is considered. For this project, ALMA will be able to provide detailed predictions of the turbulent flow field due to its ability to a) resolve small scale turbulent features and b) model the transient pressure pulse. This capability will be unique amongst CFD simulations, will be a sea change in the fidelity of multiphysics model, and will be able to capture data that is not possible to capture experimentally by exploiting the massive computing power available within the OLCF. Future work may be able model fluid-structure interactions (FSI), two-phase flow, and cavitation activity directly in order to add additional physical realism, but they are beyond the scope of this current effort.

This work will produce significant scientific impact in two distinct ways. First, improved understanding of the SNS target will allow for improved designs, greater physical insight to diagnostics, and improved prognostic capabilities which will enable more reliable facility operation. Reliable facility operation is important because the SNS is such a large scientific user facility providing unique capabilities. Additionally, the reliable and improved performance of the SNS will help it remain competitive against new foreign facilities, like the European Spallation Source. Secondly, the developed simulation tool will provide a new capability which does not exist currently, the ability to accurately simulate transient pressure phenomena in complex internal flows at fine scales. Studies of cavitation driven from transient pressure phenomena are not available in open literature despite their need amongst pulsed neutron sources, accelerator driven systems (fission reactors), and their potential in liquid walls for fusion reactors.

2 Research Objectives and Milestones

2.1 Goals of the proposed work

A one-year project is proposed, comprising **capability computing** simulations of the pressure wave induced in the flowing mercury of the Spallation Neutron Source target. The total request for this proposal is **812k node-hours on Summit**, with all simulations requiring **44% of the system**. The spatial resolution and high physics fidelity demands of these simulations require the leadership scale capabilities of the fluid solver ALMA. This research effort focuses upon using a compressible fluid simulation of liquid mercury, along with experimentally accurate thermodynamic properties, to understand the mechanics of pressure wave generation and the origins of cavitation when subjected to rapid energy deposition. The milestones and the use of requested resources are summarized in Table 1 and further explained in detail below. Note that the time required for data analysis and postprocessing following each milestone is included in the time-scale estimate.

The milestones in Table 1 are listed in order of scientific priority and importance to the project, with milestone 1 being required for all subsequent milestones. The power study, consisting of milestones 2 and 3 is of higher scientific impact than the successive wave interactions proposed for milestone 4.

2.2 Milestone details and use of requested resources

Milestone 1: Establishing bulk flow of Hg in SNS target geometry

Table 1: Summary of research milestones and use of requested Summit resources for each stage.

Mile-stone	Summit node-hrs	Time scale	Project months	Research Goal
1	18.2k	1 mo.	1	Establishing bulk flow of Hg in SNS target geometry
2	132k	3 mo.	2-4	Modeling the pressure wave from a single pulse at nominal power
3	396k	6 mo.	4-9	Examining cavitation dependence on input pulse power
4	265k	4 mo.	9-12	Modeling pressure wave interactions from a series of pulses
	1k	–	–	Data analysis and postprocessing
Total	812.2k	12 mo.		

This milestone establishes the initial condition of the mercury flow field within the SNS target geometry in the absence of inputted power. The mercury flows at a very low velocity of approximately 2 m/s, set to match experimental values at the inlet and outlet of the target. This allows us some leeway in relaxing the timestep requirements for the computations. The flow will be simulated for sufficient time (approx. 2 sec of simulation time) to allow for transients to subside throughout the entire target geometry. No proton beam pulses will occur during this time, allowing for a larger simulation timestep. The high spatial resolution of 125-200 μm will be used for this and all production simulations, and requires 2048 Summit nodes to cover the power deposition region of the SNS target. The results of this simulation will be used as the initial flow conditions for all subsequent simulations. The authors aim to achieve this milestone within the first month of the project.

A single simulation requiring 2048 Summit nodes (with a relatively large timestep) for 2 simulation seconds, taking approximately 8 wall-clock hrs. This totals to approximately 16k Summit node-hours.

Milestone 2: Modeling the pressure wave from a single pulse at nominal power

This milestone is designed to verify the spectral properties of the simulated pressure wave as it impacts the target vessel with experimental data obtained from a single proton beam pulse. The simulation will use the initial flow conditions from Milestone 1 and include a single pulse which has a duration of 700 ns, at nominal power of 2 MW, and the subsequent wave reflections throughout the target, totalling approximately 20 ms. The detailed shape of the volumetric heat deposition is known from radiation transport simulations, and is included as a time dependent source term to the internal energy as detailed in Section 3.2.3. A two-tiered timestep will be used: a smaller timestep to capture the rise and fall dynamics of the power deposition, and a larger one for the bulk wave propagation.

Our preliminary studies indicate a shock wave traveling at approximately Mach 1.2 will be generated ($c_{Hg} \approx 1450$ m/s), and that the resultant pressure drop caused by the rapid mercury expansion is highly dependent upon the modeled viscosity. It is for this reason that we are including an empirical model of mercury's viscosity (as well as thermal conductivity) that includes temperature dependence [27, 28].

A multi-timestep simulation requiring 2048 Summit nodes, broken into two steps. The first 100 μs of simulation time with a fine (short) timestep and the subsequent 17 ms of simulation time with a coarse (longer) timestep. This totals 132k Summit node-hours

Milestone 3: Examining cavitation dependence on input pulse power

The effect that the magnitude of the inputted beam power has on cavitation in the liquid mercury will be studied. Beginning with the initial flow condition established in Milestone 1, three additional beam powers will be investigated: 1.0 MW, 1.4 MW, and 2.8 MW. Experimental strain data on the target exists for the lower two of these powers, while a simulation of the greatest power level is predictive. Understanding the origins of, and ultimately preventing, cavitation is crucial to extending the lifetime of the SNS target; the amplitude of the pressure drop that is responsible for cavitation is dependent upon the beam power. Simulations will be performed to capture one pulse cycle, covering approximately 20 ms of simulation time. With the inclusion of these simulation results, local cavitation likelihood (pressure profiles) information and its dependency on input power will be obtained for use in enhanced designs to mitigate cavitation damage. Since this Milestone is only dependent upon Milestone 1, it could potentially begin earlier in the project calendar, dependant upon availability.

Three simulations at different beam input powers, of a single beam pulse each for approximately 17 ms of simulation time, totaling 396k Summit node-hours.

Milestone 4: Modeling pressure wave interactions from a series of pulses

The purpose of this milestone is to directly simulate the effects of repeated energy deposition pulses on cavitation inception. Typical operation of the SNS is with a pulse rate as high as 60 Hz. Although the wave speed is quite large relative to the size of the target and the pulse rate, the persistence time and extent of low pressure regions remains an open question. These are potentially caused by interactions of the pressure wave with the asymmetric bulk flow and turbulence regions of the target chamber.

This simulation is designed to extend the Milestone 2 simulation to include two additional sequential pulses at 60 Hz of the nominal power (2 MW) proton beam, for a total of approximately 50 ms of simulated SNS operation time (33 ms for this Milestone after the initial 17 ms of Milestone 1). Work on this milestone is therefore scheduled to occur immediately after Milestone 2, and is estimated to take 4 months to complete.

Additional multi-timestep simulations, requiring 2048 Summit nodes and building upon the simulation results from Milestone 2, of 33 ms of additional simulation time totalling 265k Summit node-hours.

2.3 Validation of single pulse strain data

Data collected from milestone two will be utilized to compare computed pressure fields on the vessel inner wall to measured strain data collected from target diagnostic runs as well as predictions from the solid model built within ABAQUS. Data will be validated against existing data by measuring the magnitude of the pressure field, frequency response of the pressure on the vessel walls, and areas of peak pressure. Pressure data may be mapped to a FEA model to compute predicted strain from the simulated pressure values. Insight will be drawn from the relative deviations of the computed values from the measured strain values and values computed within solid models. If the computed pressure field more closely aligns with the measured values without model calibration, the effects of the fluid flow can be identified as critical to the accurate prediction of the pressure propagation for the SNS target. Then, analysis of time accurate data of the pressure evolution on key target planes along with turbulent statistics will help identify the flow properties responsible for these effects.

The collection of data from milestone two will be instrumental in extending CFD simulations of the SNS target to the time-accurate regime to understand the beam's effect on the target flow as well. Due to computational limitations with commodity scale computing systems, time-accurate simulations have never before been possible of the target. This, coupled with the resolution to resolve turbulent structures within the target, will provide invaluable insight and data into validating CFD simulation assumptions regarding the turbulent energy within the target and its resulting impacts on target temperatures. This data can be utilized to tune the turbulent Prandtl number in daily analysis activities to build better models of the target. These models are critical to establishing the limits of the target operation with regards to minimum flow rates and thermal cycle fatigue.

2.4 Improved empirical model parameters for target prognostics

Data from milestones 3 and 4 will help build better prognostics tools to predict target performance as it is extended from 1.4 to 2 MW. Existing tools are built of operating data at significantly lower power levels and show strong scaling of cavitation erosion with operating power. Understanding the effects of pulse power and pule-to-pulse interaction will help tune solid models of the target performance as well as empirical models for cavitation erosion [29].

2.5 Subsequent simulations using these results

Results obtained from the high-resolution simulations described in milestones 1 to 4 will provide essential new data to explore several other parameters of importance such as the determination of local time scales, length scales and density changes. Density changes will provide insight into cavitation prone areas in the flow.

A second study of importance using these type of high resolution results will be aimed to quantify the effect of pressure fluctuations propagation in locations far away from the beam interaction area in an effort to emulate the integral effect of averaged quantities -such as attenuated fluctuation amplitudes- on typical monitoring instrumentation such as pressure transducers. The SNS has no instrumentation in the target module due to the extreme harsh environmental conditions nature of the system. Therefore, inference of the quantities of interest from instrumentation located away from the target module can be explored by back-reconstructing pressure amplitudes obtained from the high resolution simulations.

A wave propagation mitigation strategy that has been implemented at the SNS facility is the injection of helium microbubbles. This strategy has been in place for different target designs and has proven to be an effective way to limit damage to the target vessel due to cavitation erosion. Nevertheless, the detailed physical mechanisms enabling these results are not entirely understood. Therefore, the next step forward will be using simulations described in milestones 1 to 4 to provide enough spatial and temporal resolution to determine local turbulence parameters that will allow the quantification of local forces acting on over-imposed helium bubbles. In this case, the previously obtained microbubble size (spherical shape) distribution will be assumed static with respect to the pressure wave propagation velocity. Then the local parameters acting on the bubble will be calculated to provide a probability of interaction for the bubble. These types of calculations are necessary for bubble dynamics studies. Higher-order interactions will be disregarded for this study, but the track of the energy dissipated per bubble will be quantified.

3 Computational readiness

In preparation for the exascale era of computing, General Atomics has been developing an Anti-symmetric, Large-Moment, Accelerated (ALMA) fluid solver specifically designed to solve challenging problems with high physics fidelity and numerical stability at the largest scales available [22]. Detail of the requested resources for this application, the computational approach and parallel performance of ALMA are presented here.

3.1 Use of resources requested

The computational domain is a rectangular region that extends just beyond the nose section of the SNS target, and is shown in Figure 2. The computational domain extends just beyond the target's physical dimensions so that the fluid boundary is given by the target wall. The incident proton beam defines the $-z$ direction, with x and y forming a right-handed coordinate system oriented as in Figure 2, with the origin defined where the proton beam enters the target chamber (upper-left of Figure 2).

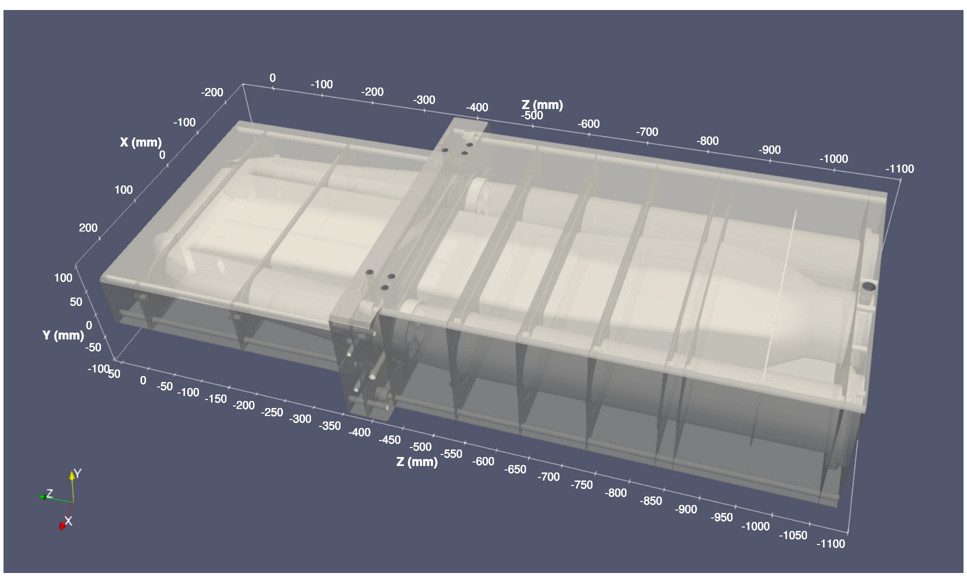

Figure 2: The SNS target chamber surrounded by the computational domain. The proton beam is incident from the coordinate origin (upper-left of the image) and proceeds in the $-z$ direction (towards the lower right). The mercury enters the chamber from two ports along the x-axis at the $-z$ location (lower-right in the Figure) and flows in the $+z$ direction until the two flows meet and reverse to flow back co-directional with the incident proton beam along the target's z-axis, until exiting the target chamber.

Table 2: Detail of physical simulation domain dimensions (used for all production runs).

Dim.	Domain (cm)	Resolution (μm)	Points per dim.	Points per MPI rank	MPI ranks per dim.
x	41.2	~ 201	2048	64	32
y	12.8	125	1024	128	8
z	111.2	~ 181	6144	64	96
total	$0.0586\ m^3$	$4.5 \times 10^{-3}\ mm^3$	1.288×10^{10}		24576

Details of the physical and simulation dimensions and their decomposition are given in Table 2. Note that the same computational domain is used for all production runs of Milestones 1-4. The simulation domain is decomposed into 24576 MPI ranks which will be distributed over 2048 Summit nodes via 12 ranks per node. Initial scaling studies confirm that such sizes ($64 \times 128 \times 64$ simulation points per MPI Rank) are capable of fitting entirely in GPU memory, and that oversubscribing 2 MPI ranks per GPU is more efficient than using a single rank per GPU.

Establishing the initial flow conditions of mercury in the target vessel is Milestone 1. This flow will be less than 2 m/s, and a total simulation time of 2 seconds is used allow for initial transients to pass. A relatively large timestep (dt= $5 \times 10^{-5} s$) can be used, resulting in 40,000 timesteps for Milestone 1. With a physical domain of 2048 nodes and using the benchmark data from Figure 3 to relate wall simulation time steps to wall clock time, this simulation is estimated to require

$$2048 \text{ Summit nodes} \times 40{,}000 \text{ timesteps} \times 0.71 \text{ Wall-clock sec per timestep} = 16.2k \text{ Summit node-hours}$$

We added an additional hour of simulation time (2k node-hours) to account for the initial parsing of the target geometry file at this scale and creation of the domain boundaries, resulting in the $18.2k$ Summit node-hours requested for Milestone 1. This domain information is propagated to subsequent simulations via the restart file. Note that at this maximum flow rate and chosen timestep, the Courant–Friedrichs–Lewy (CFL) condition is less than one.

$$CFL = v_{\max}\frac{dt}{dx} = 2\ m/s\frac{5x10^{-5}\ s}{1.25 \times 10^{-4}\ m} = 0.8$$

Milestone 2 simulates the mercury response to a single proton pulse and subsequent inter-pulse interval. The proton beam is a short-lived pulse, repeating at a frequency of 60 Hz. A single pulse deposits all of its energy in 700 ns, and the resultant pressure wave travels at approximately 1700 m/s ($\approx$ Mach 1.2) through the mercury. The speed of sound in mercury at this temperature range is about 1450 m/s, and timesteps are chosen so that the CFL condition is still comfortably satisfied for flow speeds up to Mach 1.4 (not shown). In order to capture any dynamical effects of the rise and fall characteristics of the incident beam, a shorter integration time step is used for the first 100 μs, followed by a longer time step for the remaining inter-pulse duration of 16.567 ms. This is detailed in Table 3, where the wall-clock seconds per timestep is taken from the benchmark data shown in Fig. 3. The single pulse simulation time estimates from Table 3 can then be used to calculate the total resource estimates for the different Milestones given in Section 2, where all simulations are over 2048 Summit nodes. These calculations are summarized below in Table 4.

Table 3: Estimation of simulation timesteps required for a single pulse and inter-pulse interval.

Run	Simulation timestep (s)	Simulation time (ms)	Number of timesteps	Wall-clock sec. per timestep	Wall-clock hours
1	$2x10^{-9}$	0-0.1	50,000	0.71	9.9
2	$6x10^{-8}$	0.1-16.667	276,117	0.71	54.6
	total	16.667	326,117	0.71	64.5

Table 4: Detailed estimation of simulation resources for Milestones.

Milestone	Number of pulse powers	Number of pulses	Summit node-hours
1	0	0	2048 nodes$\times$ $(8+1)$ hrs = 18.2k
2	1	1	$1 \times 1 \times$ 2048 nodes $\times$64.5 hrs = 132.1k
3	3	1	$3 \times 1 \times$ 2048 nodes $\times$64.5 hrs = 396.3k
4	1	2	$1 \times 2 \times$ 2048 nodes $\times$64.5 hrs = 264.2k
total			811k Summit node-hours

3.2 Computational approach

ALMA is based upon an anti-symmetric fluid formalism to express the fluid equations, one that obtains improved stability and results in exact conservation of relevant quantities independently of the chosen numerical scheme [22]. The ALMA code is written in Fortran object-oriented paradigm which uses the MPI library for distributed memory support, in addition to OpenMP and OpenACC directives for acceleration on CPUs and GPUs respectively. Fundamental tasks such as calculation of gradients, ghost exchanges, time integration, and vector calculus operations are performed by individual Fortran classes, which collectively constitute a model-independent library that ALMA is build upon. This library is then used to construct application-specific code by modelling its physics on the right-hand-side of the equations, in addition to describing the input parameters and setting up relevant diagnostic variables for postprocessing. The most recent version of ALMA has been used to built three physical models namely, the Navier-Stokes equations, Magneto-Hydrodynamics equations, and the Braginskii equations. The proposed simulations use the Navier-Stokes equations. The Navier-Stokes equations are written using a time derivative that includes an anti-symmetric flow operator: $\partial_t + 1/2\,(\nabla\cdot\mathbf{v}+\mathbf{v}\cdot\nabla)$, acting upon generalized fluid moments (fields) $\sqrt{\rho}, \sqrt{\rho}\mathbf{v}, \sqrt{U}$. The fluid equations in anti-symmetric form are shown in Eqs. (A.12) to (A.14) in Appendix A of Ref. [22].

The square of the generalized fluid moments: mass, momentum, and internal energy per unit volume (respectively), then trivially preserve positivity, $\rho = (\sqrt{\rho})^2, \mathbf{p} = \left(\sqrt{\rho}\right)^2\mathbf{v}, U = (\sqrt{U})^2$. More importantly, time evolution using the anti-symmetric flow operator and a centered implicit scheme can be shown to be exactly conservative and unconditionally stable, regardless of the spatial discretization employed. This makes the fluid model amenable to simple stencil methods (finite differences) and domain decomposition. This formalism allows a simple, robust, and scalable implementation using finite differences on regular grids, which involve only point-to-point communication and ports well to GPU architecture. Other thermodynamic state variables (such as pressure and temperature) are derived from the generalized fluid moments in conjunction with the equation of state for liquid mercury, which is detailed in Sec. 3.2.2.

We aim to use the MPI-OpenACC parallelization strategy, wherein MPI is used for domain decomposition across nodes and OpenACC is used for GPU offloading. Although ALMA possess OpenMP directives to leverage CPU cores for speedup, the GPU-accelerated kernels are far superior in performance (after considering data movement from and to the host) and hence are advocated in these simulations. The requisite libraries to compile the code are available on the Summit cluster. The code performance estimates obtained from a benchmarking study OLCF's Summit supercomputer are provided in Sec. 3.3.

As mentioned in Sec. 1, previous computations with liquid mercury have used the pressure-based solver on account of incompressible flow approximation [11–13]. ALMA on the other hand considers the working fluid to be at least weakly compressible, and solves the mass, momentum, and energy conservation equations simultaneously (in an anti-symmetric formulation.) This compressible formulation allows coupling of temperature and velocity, which is especially important to account for local changes in the flowfield triggered by the rapid heating of liquid mercury ($\sim 10^7$ K/s).

3.2.1 Data Sampling and Postprocessing

This section elaborates the data sampling procedure and the concomitant memory requirements, as well as data analysis techniques used to derive meaningful results from the computations. We plan to extract data in double precision floating point accuracy on 6 two-dimensional planes: two x–y planes at $z = -50, -25$ cm, two x–z planes at $y = 0$ m and $y = 6.4$ cm, and two y–z planes at $x = 0, 20.6$ cm. Our approach to data sampling during the simulations is based on the ongoing physics in the SNS target. The primary constraint for the sampling frequency comes from the rapid heat deposition, which lasts for 700 ns, which then begets a pressure wave travelling at Mach ≈ 1.2. Referring to Table 3, the aforementioned phenomena will most likely occur during Run 1 wherein the simulation time-step is ~ 2 ns. In order to capture the resultant dynamical effects with sufficient time-resolution, we plan to sample data once every 50 iterations on the two-dimensional planes, which translates to a sampling frequency of 1 MHz and 1000 samples.

Table 5: Data sampling details and estimated amounts for a simulation of 1 proton beam pulse.

Planes	**Location** (cm)	**# Points**	**Required memory (GB) =** $N_x \times N_y \times N_z \times$**nvar**$\times N_{\mathbf{samp}} \times$**bytes/float**
x–y	$z = -50$	2048×1024	$2048 \times 1024 \times 1 \times 5 \times 1552 \times 8 \approx 130.19$
x–y	$z = -25$	2048×1024	$2048 \times 1024 \times 1 \times 5 \times 1552 \times 8 \approx 130.19$
y–z	$x = 0$	1024×6144	$1 \times 1024 \times 6144 \times 5 \times 1552 \times 8 \approx 390.57$
y–z	$x = 20.6$	1024×6144	$1 \times 1024 \times 6144 \times 5 \times 1552 \times 8 \approx 390.57$
x–z	$y = 0$	2048×6144	$2048 \times 1 \times 6144 \times 5 \times 1552 \times 8 \approx 781.15$
x–z	$y = 6.4$	2048×6144	$2048 \times 1 \times 6144 \times 5 \times 1552 \times 8 \approx 781.15$
x–y–z	–	$2048 \times 1024 \times 6144$	$2048 \times 1024 \times 6144 \times 5 \times 2 \times 8 \approx 1030.79$
Restart	–	$2048 \times 1024 \times 6144$	$2048 \times 1024 \times 6144 \times 9 \times 1 \times 8 \approx 927.71$
Total			≈ 4.57 TB

For the inter-pulse simulation (Run 2), the sampling frequency is reduced by a factor of 10 to 100 kHz (data sampled once every 500 iterations), which results in about 552 samples. Hence a total 1552 samples are generated from both the runs. In addition to two-dimensional planes, we also plan to extract one instance of the entire three-dimensional flowfield during each run. For data extracted on the wall, all the three components of skin-friction coefficient, pressure, and heat transfer magnitude are examined. The pressure distribution is especially important as it will be used to compute strain data on the vessel for validation purposes. For data on the mid-planes and three-dimensional flowfields, all the three components of the velocity vector, density, and temperature are measured. In all the cases, a sum total of five quantities are written in the HDF5 file format with the exception of the restart file wherein the code needs to preprocess nine quantities before resuming the simulations. Using this information, the overall estimate of the memory required to sample data for the duration of 1 pulse is shown in Table 5.

We plan to post-process data corresponding to one single run (with or without pulsing) and archive it on Summit's HPSS archive, before proceeding to the next case. Files generated from the data analysis procedure will be transferred to the in-house cluster at General Atomics. The data analysis procedure roughly involves the following steps, enumerated in the increasing order of sophistication:

1. Compute first and second order statistical moments. Compare results with existing RANS simulations and experimental data.
2. Delineate time- and length-scales using Fourier transforms and note down peak frequencies.
3. Investigate the causes of cavitation inception using statistical estimates of correlations, especially due to the quasi-streamwise vortices mentioned briefly in Sec. 1.
4. Use Reduced Ordered Modelling techniques such as Dynamic Mode Decomposition to perform a rank-based decomposition of the flowfield into dynamically significant modes.

The steps above will be performed by an in-house suite of Fortran codes, with MPI and OpenMP support to handle large files. Prior to using these codes, the HDF5 result files are converted to a simple unformatted binary file with a customized header that provides information on the type of plane (xy,yz,xz), number of grid points, time-step, and freestream quantities. These aspects are encapsulated in a Python wrapper that provides a simplified interface to perform any of the steps mentioned above. Based on the scaling data of the analysis codes on other clusters (not shown here), we expect the current problem size to run efficiently on 4 Summit nodes (5 MPI ranks + 4 OpenMP threads). A rough estimate of 1k node-hours mentioned in Table 1 will enable us to perform about 250 calculations in total, each with a wall-time of 1 hour.

3.2.2 Computational modeling of liquid mercury

The behaviour of liquid mercury at room temperature deviates significantly from ideal gas behaviour, as indicated by its compressibility factor $Z = 3.7$ ($Z \approx 1$ for ideal gas). The equation of state used in the simulations is reproduced from the work of Kuchhal et al. [30] and is shown in Eq. (1):

$$\begin{aligned} \frac{V(P,T)}{V(0,T_R)} &= \frac{\rho(0,T_R)}{\rho(P,T)} = \left((1+\beta)\exp\left(Z\left[P-\xi\left(T-T_R\right)\right]\right)-\beta\right)^{-1/\eta} \\ \beta &= B'_T(0,T_R)\,/\,\left[B_T(0,T_R)\,Z\right]; \quad \eta = B'_T(0,T_R)+B_T(0,T_R)\,Z \end{aligned} \tag{1}$$

where $T_R = 313.65\,\mathrm{K}$, $B_T(0, T_R) = 24.29\,\mathrm{GPa}$, $B'_T(0, T_R) = 10.04$, $Z = 164.951 \times 10^{-3}\,\mathrm{GPa}^{-1}$, $\alpha(0, T_R) = 1.82 \times 10^{-4}\,\mathrm{K}^{-1}$ and $\rho(0, T_R) = 13.495\,\mathrm{g/cc}$ are material-specific constants (see Table I in that reference). The experimental data of Ayrinhac et al. [31] agrees well with the curve described by Eq. (1) and a plot is available on request, which has been omitted for space.

In addition to the equation of state, temperature variation of transport properties of liquid mercury viz. dynamic viscosity (μ) [27] and thermal conductivity (k) [28] are also modeled in the code. Their respective expressions are given in Eq. (2),

$$\log\mu = A + B/(C - T); \quad k/k_0 = (T/T_0)^{0.75} \tag{2}$$

where $A = -3.1105$, $B = -51.209$, and $C = 124.04$ are constants specific to liquid mercury, T is the absolute temperature in K, and k_0 is the thermal conductivity at the lowest available temperature, T_0.

3.2.3 Heat deposition profile

Energy deposition by the proton beam creates a heat distribution on the surface of the target, which can be approximated by a super-Gaussian function on the x–y plane with exponential decay along the z-direction (see Fig. 2 for the orientation of the axes.) The corresponding expression is shown in Eq. (3),

$$Q(\mathbf{x}) = q\exp\left[-\left\{(a(x-x_c))^2 + \left(2b(x-x_c)\left(y-x_c\right)\right) + \left(c\left(y-y_c\right)\right)^2\right\}^4\right]\exp\left[-d\left(z-z_c\right)\right] \tag{3}$$

where $Q(\mathbf{x})$ is the magnitude volumetric heat deposition in J/m^3, q is the magnitude of heat added in J, x_c, y_c, z_c are the centroid coordinates of the source term, and a, b, c, d are constants tuned to fit this equation to the existing data. In order to model the pulsing nature of heat deposition, an additional sinusoidal term, $\sin\left[2\pi f(t - t_0)\right]$ is incorporated in Eqs. (3), where f is the pulsing frequency, t is the elapsed time, and t_0 is the time at which the heating commences.

3.3 Parallel performance

The ALMA fluid simulation framework was designed to take advantage of GPU architecture, starting with the uniform cartesian grid domain and finite difference stenciling, memory may be efficiently addressed via complex indexing, rather than be dependent upon the local geometry which results in divergent calculations on adjacent threads. A focus on relatively small memory footprint to maximize thread occupancy and only nearest-neighbor communications.

The parallel scaling performance of ALMA has been benchmarked on up to 4096 nodes of OLCF Summit. The wall-clock per timestep value used for the resource calculations in Tables 3 and 4 are based on estimates from simulations that represent the full computational complexity of the production runs proposed here, and are shown in Figure 3. This include the anti-symmertric Navier-Stokes equations with the mercury equation of state (Section 3.2.2) and temperature dependent viscosity. They include the boundary condition evaluations at the fluid interface with the SNS target geometry, and utilization of a flux-limiter (not described here). These benchmarks also reflect the I/O required, including mapping the target geometry to the domain grid and 2D plane data at relevant sampling rates.

Strong scaling applies to the proposed work because, together with the resolution required for the desired simulations, it informs the balance between resource demands (node-hours) and required

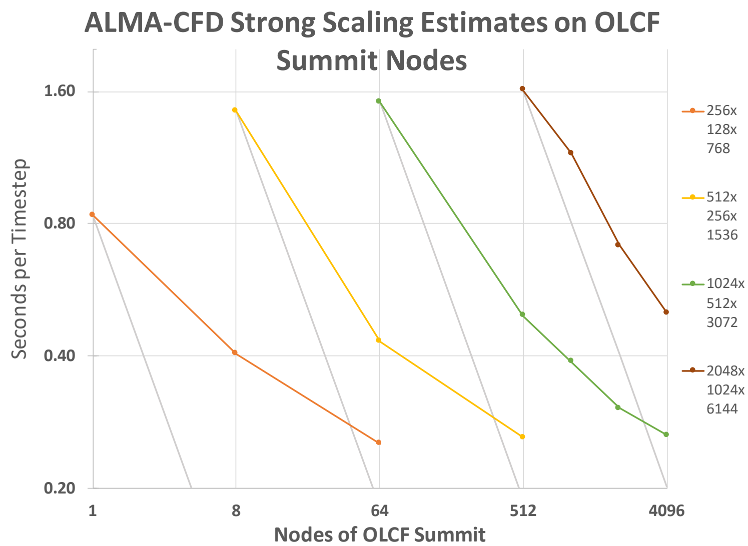

Figure 3: Strong scaling estimates of ALMA on OLCF Summit for different problem sizes, used for the resource request calculations. Ideal scaling is shown in grey. Note the degradation from ideal scaling performance typical of reduced GPU occupancy. The 2048 node implementation of the largest domain, shown here in brown (2048 × 1024 × 6144), and requiring 0.71 wall-clock seconds per timestep is chosen for the production runs requested.

wall-clock time. While the domain size for the production runs can be extended over more (4096) nodes than the 2048 that are proposed here, it is less efficient to do so, as one timestep would require 4096 nodes × 0.50 seconds = 0.57 node-hours, while restricting the simulations to 2048 nodes requires only 2048 nodes × 0.71 seconds = 0.40 node-hours in addition to retaining a manageable amount of job-maintenance in the form of sequential restarts.

3.4 Developmental work

Although the ALMA fluid simulation framework remains under active development at General Atomics, it is completely capable of performing the simulations proposed in this project now, without any additional modifications. The project PI, M. Kostuk, is one of the original ALMA co-authors, and the project co-PI, A. Deshpande is responsible for the improved mercury equation of state, viscosity and heat deposition functionality, as well as the data postprocessing scripts. In addition, A. Deshpande has a working knowledge of ALMA, having recently contributed to more general feature enhancements.

No additional development work on ALMA is required for this project to proceed, however as the HPC software team at General Atomics is actively working on ALMA to advance goals external to this INCITE project, they are more than capable of addressing any unforeseen complications that may arise.

PERSONNEL JUSTIFICATION AND MANAGEMENT PLAN

PERSONNEL JUSTIFICATION

The collaborative team from General Atomics (GA) and Oak Ridge National Laboratory (ORNL) contain the necessary skills and expertise in both large scale numerical simulation and the physics of high power deposition in mercury to successfully carry out the proposed research into the origins of pressure-wave cavitation within the Spallation Neutron Source target. No new hires or personnel turnover is foreseen under this project. The team is comprised of:

- **Dr. Mark Kostuk** (PI) is one of the original co-authors of the ALMA fluid simulation framework that is being used to perform the production runs proposed for this project, and attended the OLCF Summit new-user training workshop in 2018. Dr. Kostuk is currently the leader of the Advanced Computing group at General Atomics.
- **Dr. Elvis Dominguez-Ontiveros** (co-PI) is the current R&D leader for thermal and fluid sciences in the Source Development Engineering group at the ORNL Spallation Neutron Source. His expertise lies in the intersection of mechanical engineering and nuclear engineering.
- **Dr. Justin Weinmeister** (co-PI) is an expert in fluid mechanics and the SNS target: He has supported fluids R&D activities for the SNS target for the previous four years and is currently a technical staff engineer at ORNL.
- **Dr. Akshay Deshpande** (co-PI) is an ORAU Postdoctoral Scholar in the Advanced Computing group at General Atomics, working on the development of the ALMA code.

MANAGEMENT PLAN

The point of contact for the overall project and the ALMA fluid dynamic solver is Dr. Kostuk, whose email is kostukm@fusion.gat.com , while the point of contact for the SNS is Dr. Dominguez-Ontiveros, whose email is dominguezoee@ornl.gov. We anticipate having regularly scheduled group meetings to discuss the general project progress and the individuals' contributions to it.

- **Dr. Mark Kostuk** is responsible for the overall project completion, communication and ultimate success. He will verify the performance of ALMA and be the lead developer should any unforeseen problems arise. He will execute some of the ALMA simulation runs and will assist in writing manuscripts for publications that result from this project, including sections specific to the software and production run details. He will disseminate major project achievements.
- **Dr. Elvis Dominguez-Ontiveros** will coordinate the communication between the ORNL team and the GA researchers to provide prompt and adequate information about the relevant physics requirements for the simulations. He will assist in preparing and releasing proper documentation for dissemination to the scientific community. He will help with selecting, processing, and formatting validation data.
- **Dr. Justin Weinmeister** will support GA researchers and ORNL lead Dr. Dominguez-Ontiveros with SNS target data and provide area-of-expertise support on modeling decisions. The necessary target data includes up-to-date computational geometry models, boundary conditions, historical operating data, and validation data sets.
- **Dr. Akshay Deshpande** will assist Dr. Mark Kostuk in monitoring the SNS target simulations on Summit. Following the simulations, he will use the in-house Fortran codes to perform tasks entailed in the data analysis procedure (see Sec. 3.2.1) to extract physically-meaningful results.

MILESTONE TABLE

Proposal Title : Cavitation inception in turbulent liquid metal

Year 1 of 1

Milestone	Details	Dates	Status (renewals only)
1	**Resources:** Summit **Node hours: 18.2k** **Filesystem storage (TB and dates):** 1 TB, 0–12 **Archival storage (TB and dates):** 1 TB, 0–12 **Software Application:** ALMA **Tasks:** Establish initial Hg flow rate using a single production run on 2048 nodes; stored for remainder of project **Dependencies:** none	0–12	n.a.
2	**Resources:** Summit **Node hours: 132k** **Filesystem storage (TB and dates):** 6 TB, 2–4 **Archival storage (TB and dates):** 6 TB, 2–12 **Software Application:** ALMA **Tasks:** Validation of a single pulse-induced pressure wave at nominal power using a single simulation (3 restarts) on 2048 nodes. **Dependencies:** 1	2–4	n.a.
3	**Resources:** Summit **Node hours: 396k** **Filesystem storage (TB and dates):** 16 TB, 4–9 **Archival storage (TB and dates):** 21 TB, 4–12 **Software Application:** ALMA **Tasks:** Validation and prediction of the input power on cavitation, using a series of 3 production runs (3 restarts ea.) on 2048 nodes at different beam powers, including one that has not been tested experimentally. **Dependencies:** 1	4–9	n.a.
4	**Resources:** Summit **Node hours: 265k** **Filesystem storage (TB and dates):** 11 TB, 9–12 **Archival storage (TB and dates):** 31 TB, 9–12 **Software Application:** ALMA **Tasks:** Exploration of the cavitation induced from interactions of multiple successive pressure waves, using a single simulation (6 restarts) extending that of Milestone 2. **Dependencies:** 2	9–12	n.a.

PUBLICATIONS FROM PRIOR INCITE AWARDS

As this is a new INCITE proposal, no publications from prior incite awards exist.

Curriculum Vitae

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PROFESSIONAL PREPARATION

PhD, Physics, University of California, San Diego CA (2012)
MS, Physics, University of California, San Diego CA (2008)
BS, Chemistry and Physics, Union College, Schenectady NY (2001)

APPOINTMENTS

2021–present: Manager of Advanced Computing, General Atomics: Magnetic Fusion Energy.
2015–2021: Computational Physicist, General Atomics: Magnetic Fusion Energy.

FIVE PUBLICATIONS MOST RELEVANT TO THIS PROPOSAL

1. Halpern F, Sfiligoi I, Kostuk M, Stefan R, Waltz R. Simulations of plasmas and fluids using anti-symmetric models. Journal of Computational Physics. 2021 November; 445:110631-. Available from: https://linkinghub.elsevier.com/retrieve/pii/S002199912100526X DOI: 10.1016/j.jcp.2021.110631
2. Kostuk M, Uram T, Evans T, Orlov D, Papka M, Schissel D. Automatic Between-Pulse Analysis of DIII-D Experimental Data Performed Remotely on a Supercomputer at Argonne Leadership Computing Facility. Fusion Science and Technology. 2018 February 01; 74(1- 2):135-143. Available from: https://www.tandfonline.com/doi/full/10.1080/15361055.2017.1390388 DOI: 10.1080/15361055.2017.1390388
3. Jouzdani P, Bringuier S, Kostuk M. A method of determining molecular excited-states using quantum computation. MRS Advances. 2021 July 26; 6(22):558-563. Available from: https://link.springer.com/10.1557/s43580-021-00111-3 DOI: 10.1557/s43580-021-00111-3
4. Sammuli B, Barr J, Eidietis N, Olofsson K, Flanagan S, Kostuk M, Humphreys D. TokSearch: A search engine for fusion experimental data. Fusion Engineering and Design. 2018 April; 129:12-15. Available from: https://linkinghub.elsevier.com/retrieve/pii/S0920379618301042 DOI: 10.1016/j.fusengdes.2018.02.003
5. Meneghini O, Smith S, Snyder P, Staebler G, Candy J, Belli E, Lao L, Kostuk M, Luce T, Luda T, Park J, Poli F. Self-consistent core-pedestal transport simulations with neural network accelerated models. Nuclear Fusion. 2017 August 01; 57(8):086034-. Available from: https://iopscience.iop.org/article/10.1088/1741-4326/aa7776 DOI: 10.1088/1741-4326/aa7776

RESEARCH INTERESTS AND EXPERTISE

Dr. Kostuk leads the Advanced Computing team at General Atomics. His primary research interest is on the optimization and data assimilation of chaotic physical systems using high performance computing (HPC) techniques. This is expressed through work on high fidelity numerical algorithms, solution methods, and their efficient realization on leadership class hardware. During his doctoral work, Dr. Kostuk developed methods of nonlinear-model estimation, Bayesian optimization, and uncertainty quantification of high dimensional chaotic systems. At General Atomics, he has been applying his 15 years of GPU and HPC software experience to various plasma simulation codes, and is a co-author of the ALMA fluid simulator. As an active and dedicated member of the fusion community, Dr. Kostuk presented a novel HPC application in support of fusion experimental research at the 2017 IAEA-TM on Data Analysis and Processing, and is presenting current work in quantum computing methods at the 2021 PFMC-18 conference on plasma facing materials. With interests in all types of advanced computing, he is an active user at NERSC, Argonne and Oak Ridge Leadership Computing Facilities, is a regular participant at GPU hackathons and was instrumental in GA obtaining membership into the IBM Q-Hub network for quantum computing.

SYNERGISTIC ACTIVITIES

1. DOE/FES: Quantum Computing for Fusion Energy Materials (PI 2019-present)
2. AToM DOE/SC SciDAC: Advanced Tokamak Modeling (co-PI 2017-2021)
3. DOE/SC SciDAC: Theory and Simulation of Fusion Plasmas (Researcher on 2019 supplement with ALMA)
4. DIII-D National Fusion Facility: Computer Systems and Science Group

COLLABORATORS In addition to other employees of General Atomics Magnetic Fusion Energy

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Noel, Thomas, ColdQuanta
Orlov, Dmitry, University of California, San Diego
Papka, Michael, Argonne National Laboratory
Pelton, Sabine, University of Central Florida
Pointer, David, Oak Ridge National Laboratory
Safro, Ilya, University of Delaware
Sfiligoi, Igor, University of California, San Diego
Snyder, Philip B., Oak Ridge National Laboratory
Stefan, Ryan, Callaway Golf Company
Suchara, Martin, Amazon
Uram, Thomas, Argonne National Laboratory
Whiteley, Samuel, HRL Laboratories

Curriculum Vitae
Elvis Dominguez-Ontiveros
dominguezoee@ornl.gov | (865) 574-8319

PROFESSIONAL PREPARATION

PhD, Mechanical Engineering, Texas A&M University (2010)
MS, Nuclear Engineering, Texas A&M University (2004)
BS, Electrical Engineering, Instituto Politecnico Nacional (IPN) Mexico (2000)

APPOINTMENTS

2020–present, Sr. R&D Staff at Spallation Neutron Source ORNL
2015–2020, R&D Staff at Advanced Reactor Engineering ORNL
2010–2015, Research Engineer at Nuclear Engineering Texas A&M University

FIVE PUBLICATIONS MOST RELEVANT TO THIS PROPOSAL

1. Barbier, C, Dominguez-Ontiveros, E, & Sangrey, R. "Small Bubbles Generation With Swirl Bubblers for SNS Target." Proceedings of the ASME 2018 5th Joint US-European Fluids Engineering Division Summer Meeting. Montreal, Quebec, Canada. July 15–20, 2018. V003T20A001. ASME. https://doi.org/10.1115/FEDSM2018-83077
2. Emilian Popov, Lilin He, Elvis Dominguez-Ontiveros, and Yuri Melnichenko, Detection of vapor nanobubbles by small angle neutron scattering (SANS), Applied Physics Letters, 112,153704 (2018), https://doi.org/10.1063/1.5023595
3. F. Rasheed, E. Dominguez-Ontiveros, J. Weinmeister, and C. Barbier, Deep Learning for Intelligent Bubble Size Detection in the Spallation Neutron Source Visual Target, Proceedings of the 2020 ASME International Mechanical Engineering Congress and Exposition, 10: V010T10A001 (2020), https://doi.org/10.1115/IMECE2020-23164.
4. Barbier, C, & Dominguez-Ontiveros, E. "Improving Computational Fluid Dynamics Simulations for the Spallation Neutron Source Jet-Flow Target." Proceedings of the ASME 2016 Fluids Engineering Division Summer Meeting collocated with the ASME 2016 Heat Transfer Summer Conference and the ASME 2016 14th International Conference on Nanochannels, Microchannels, and Minichannels.Washington, DC, USA. July 10–14, 2016. V01AT03A011. ASME. https://doi.org/10.1115/FEDSM2016-7671
5. Barbier, C., Dominguez-Ontiveros, E., Weinmeister, J., Slade, J., Ottinger, D., and Sangrey, R. (September 27, 2021). "A Compact Gas Liquid Separator for the Spallation Neutron Source Mercury Process Loop ." ASME. J. Fluids Eng. March 2022; 144(3): 031403. https://doi.org/10.1115/1.4052241

RESEARCH INTERESTS AND EXPERTISE Dr. Dominguez-Ontiveros is the current R&D leader for thermal and fluid sciences in the Source Development Engineering group at the ORNL Spallation Neutron Source. Dr. Dominguez-Ontiveros expertise lies in the intersection of mechanical engineering and nuclear engineering. He focuses on experimental and computational work related to components found in nuclear reactors and neutron production facilities. His current research focuses on

Computational Fluid Dynamics (CFD),Experimental Fluid Mechanics and heat transfer, Flow Induced Vibrations, Fluid-structure interactions, Multiphase flows, Liquid Metal coolants, Irradiation Experiments, Sensor development

SYNERGISTIC ACTIVITIES

1. SNS: Building Initial Dynamic Systems Models for Digital Twins of the Crypogenic Moderator System at the ORNL Spallation Neutron Source
2. SNS: Measurements of Bubble Production in Liquid Metal
3. SNS: Fluid-Structure-Interaction of Target Vessel with High Re number Liquid Metal

COLLABORATORS

In addition to other employees of ORNL
Richard Howard, Idaho National Laboratory, Idaho
Carlo Estrada, Idaho National Laboratory, Idaho
Kevin Chen, University of Pittsburgh, Pennsylvania
Yassin Hassan, Texas A&M University, Texas
Scott Greenwood, Modelon, Michigan
Eric Johnsen, University of Michigan, Michigan
Salome Thorson, Sandia National Laboratory, New Mexico

Curriculum Vitae

Justin Weinmeister
weinmeistejr@ornl.gov | (856) 574-8806

PROFESSIONAL PREPARATION

MS, Mechanical Engineering, Colorado State University (2018)
BS, Mechanical Engineering, Colorado State University (2017)

APPOINTMENTS

2019–present, Technical Staff Member of Nuclear Energy and Fuel Cycle Division at ORNL
2018–2019, Post-Master in Neutron Technologies Division at ORNL
2017–2018, Graduate Research Assistant of Computational Fluid Dynamics and Propulsion Laboratory at Colorado State University

FIVE PUBLICATIONS MOST RELEVANT TO THIS PROPOSAL

1. J. Weinmeister, C. Barbier, and E. Dominguez-Ontiveros, Gas Wall Layer Experiments for Spallation Neutron Source Target, Proceedings of the ASME-JSME-KSME 2019 8th Joint Fluids Engineering Conference, 3A: V03AT03A048 (2019), https://doi.org/10.1115/AJKFluids2019-5101.
2. C. Barbier, E. Dominguez-Ontiveros, J. Weinmeister, J. Slade, D. Ottinger, and R. Sangrey, A Compact Gas Liquid Separator for the Spallation Neutron Source Mercury Process Loop, ASME J. Fluids Eng. 144(3): 031402 (2022), https://doi.org/10.1115/1.4052241.
3. F. Rasheed, E. Dominguez-Ontiveros, J. Weinmeister, and C. Barbier, Deep Learning for Intelligent Bubble Size Detection in the Spallation Neutron Source Visual Target, Proceedings of the 2020 ASME International Mechanical Engineering Congress and Exposition, 10: V010T10A001 (2020), https://doi.org/10.1115/IMECE2020-23164.
4. C. Barbier, J. Weinmeister, F. Rasheed, K. Johns, D. Winder, B. Riemer, D. Ottinger, M. Costa, and R. Sangrey, Bubble Generation in the SNS 2 MW Mercury Target, IPAC 2021 - 12th International Particle Accelerator Conference, ISSN 2673-5490: 3567-3570 (2021), doi:10.18429/JACoW-IPAC2021-WEPAB367.
5. J. Weinmeister, X. Gao, and S. Roy, Analysis of a Polynomial Chaos-Kriging Metamodel for Uncertainty Quantification in Aerodynamics, AIAA Journal 57(6): 2280-2296 (2019), http://dx.doi.org/10.2514/1.J057527.

RESEARCH INTERESTS AND EXPERTISE

Computational Fluid Dynamics (CFD), Uncertainty Quantification (UQ), Verification and Validation (V&V), Design Optimization, Two-Phase Flow, Cavitation

SYNERGISTIC ACTIVITIES

1. 25% of current time supports fluid R&D activities for SNS target with current focus on collecting two-phase flow validation data

2. 25% of current time supports exploratory viscous flow modeling
3. 50% of time supports general CFD and thermal modeling applications

COLLABORATORS In addition to other employees of Oak Ridge National Laboratory

Casey J. Jesse, Idaho National Laboratory
Xinfeng Gao, Colorado State University
Stephen Guzik, Colorado State University
Nelson Xie, Colorado State University
Sourajeet Roy, Indian Institute of Technology Roorkee
Aditi Krishna Prasad, Intel Corporation

Curriculum Vitae
Akshay S. Deshpande
deshpandea@fusion.gat.com

PROFESSIONAL PREPARATION

PhD, Aeronautics and Astronautics, Purdue University (2021)
MS, Aeronautics and Astronautics, Purdue University (2017)
BTech, Mechanical and Energy Engineering, VIT University (2015)

APPOINTMENTS

2021–present, Postdoctoral Researcher at General Atomics
2017–2021, Graduate Research Assistant at Purdue University
2016–2017, Graduate Teaching Assistant at Purdue University

FIVE PUBLICATIONS MOST RELEVANT TO THIS PROPOSAL

1. A. S. Deshpande, and J. Poggie. Large-scale unsteadiness in a compression ramp flow confined by sidewalls. Physical Review Fluids, 6(2), 024610 (2021), https://doi.org/10.1103/PhysRevFluids.6.024610
2. A. S. Deshpande, and J. Poggie. Unsteady Characteristics of Compressible Reattaching Shear Layers. Physics of Fluids, 32(6), 066103, (2020), https://doi.org/10.1063/5.0008752
3. A. S. Deshpande, and J. Poggie. Flow Control of Swept Shock-Wave/Boundary-Layer Interaction using Plasma Actuators. Journal of Spacecraft and Rockets, 55(5), 1198-1207, (2018), https://doi.org/10.2514/1.A34114

RESEARCH INTERESTS AND EXPERTISE

Computational Fluid Dynamics (CFD), Compressible Flows, High Performance Computing (HPC), Statistical Analysis, Reduced Ordered Modelleing

SYNERGISTIC ACTIVITIES

1. ALMA-CFD development of new capabilities

COLLABORATORS

Kostuk, Mark, General Atomics
Poggie, Jonathan, Purdue University

References

[1] Oak Ridge National Laboratory, “Spallation Neutron Source website,” 2022. https://neutrons.ornl.gov/sns.

[2] T. E. Mason, D. Abernathy, I. Anderson, J. Ankner, T. Egami, G. Ehlers, A. Ekkebus, G. Granroth, M. Hagen, K. Herwig, J. Hodges, C. Hoffmann, C. Horak, L. Horton, F. Klose, J. Larese, A. Mesecar, D. Myles, J. Neuefeind, M. Ohl, C. Tulk, X. L. Wang, and J. Zhao, “The spallation neutron source in oak ridge: A powerful tool for materials research,” *Physica B: Condensed Matter*, vol. 385-386, pp. 955–960, 2006.

[3] D. E. Winder, “Evolution of the high-power spallation neutron mercury target at the sns,” in *Conference: 12th International Particle Accelerator Conference (IPAC)*, (Campinas, Brazil), 2021.

[4] B. W. Riemer, D. A. McClintock, S. Kaminskas, and A. A. Abdou, “Correlation between simulations and cavitation-induced erosion damage in spallation neutron source target modules after operation,” *Journal of Nuclear Materials*, vol. 450, no. 1, pp. 183–191, 2014.

[5] J. R. Haines, B. W. Riemer, D. K. Felde, J. D. Hunn, S. J. Pawel, and C. C. Tsai, “Summary of cavitation erosion investigations for the sns mercury target,” *Proceedings of the 6th International Workshop on Spallation Materials Technology*, vol. 343, no. 1, pp. 58–69, 2005.

[6] Y. Liu, W. Blokland, C. Long, S. Murray, B. Riemer, R. Sangrey, M. Wendel, and D. Winder, “Strain measurement in the recent sns mercury target with gas injection,” *Journal of Physics: Conference Series*, vol. 1067, p. 052022, 2018.

[7] H. Jiang, D. Winder, D. McClintock, D. Bruce, R. Schwartz, M. Kyte, and T. Carroll, “Quantifying the reduction in cavitation-induced erosion damage in the spallation neutron source mercury target by means of small-bubble gas injection,” *Wear*, vol. 496-497, p. 204289, 2022.

[8] B. W. Riemer, “Benchmarking dynamic strain predictions of pulsed mercury spallation target vessels,” *Journal of Nuclear Materials*, vol. 343, no. 1, pp. 81–91, 2005.

[9] L. Lin and D. Winder, “Tunable eos material model in the simulation of pulsed mercury spallation target vessel,” in *ASME 2019 Pressure Vessels & Piping Conference*, vol. Volume 4: Fluid-Structure Interaction, (V004T04A001), 2019.

[10] M. I. Radaideh, L. Lin, H. Jiang, and S. Cousineau, “Bayesian inverse uncertainty quantification of the physical model parameters for the spallation neutron source first target station,” *Results in Physics*, vol. 36, p. 105414, 2022.

[11] M. W. Wendel and M. S. Tov, “CFD analysis of a liquid mercury target for the national spallation neutron source,” Tech. Rep. CONF-970739-1, Oak Ridge National Laboratory, Oak Ridge, TN, 1997.

[12] M. W. Wendel and M. S. Tov, “CFD analysis of a liquid-mercury target for the spallation neutron source,” Tech. Rep. CONF-980606, Oak Ridge National Laboratory, Oak Ridge, TN, 1998.

[13] M. W. Wendel and J. R. Haines, “Applicability of three-dimensional CFD simulation of the spallation neutron source mercury target,” Tech. Rep. ORNL/P00-106488, Oak Ridge National Laboratory, Oak Ridge, TN, 2000.

[14] W. D. Pointer, M. W. Wendel, J. M. Crye, A. E. Ruggles, D. K. Felde, P. A. Jalouk, G. L. Yoder Jr., and J. R. Haines, "Scaled experiments and CFD simulations supporting the design of the spallation neutron source mercury target," in *ASME International Mechanical Engineering Congress and Exposition*, vol. Fluids Engineering, pp. 309–316, American Society of Mechanical Engineers, 2000.

[15] M. Wendel and J. Haines, "Cfd-based design improvements to the spallation neutron source target," in *2001 ASME Fluids Engineering Division Summer Meeting*, 2001.

[16] M. W. Wendel, P. J. Geoghegan, and D. K. Felde, "Simulation and mockup of sns jet-flow target with wall jet for cavitation damage mitigation," in *4th Joint US-European Fluids Engineering Summer Meeting*, 2014.

[17] C. Barbier, M. Wendel, D. Felde, and M. C. Daugherty, "Numerical and experimental investigation of the flow in the SNS jet flow target," in *ASME International Mechanical Engineering Congress and Exposition*, vol. Volume 7B: Fluids Engineering Systems and Technologies, American Society of Mechanical Engineers, 2015.

[18] *Improving Computational Fluid Dynamics Simulations for the Spallation Neutron Source Jet-Flow Target*, vol. Volume 1A, Symposia: Turbomachinery Flow Simulation and Optimization; Applications in CFD; Bio-Inspired and Bio-Medical Fluid Mechanics; CFD Verification and Validation; Development and Applications of Immersed Boundary Methods; DNS, LES and Hybrid RANS/LES Methods; Fluid Machinery; Fluid-Structure Interaction and Flow-Induced Noise in Industrial Applications; Flow Applications in Aerospace; Active Fluid Dynamics and Flow Control — Theory, Experiments and Implementation of *Fluids Engineering Division Summer Meeting*, 07 2016. V01AT03A011.

[19] J. Katz, "Cavitation phenomena within regions of flow separation," *Journal of Fluid Mechanics*, vol. 140, pp. 397–436, 1984.

[20] J. Katz and T. J. O'Hern, "Cavitation in Large Scale Shear Flows," *Journal of Fluids Engineering*, vol. 108, pp. 373–376, 9 1986.

[21] K. Agarwal, O. Ram, and J. Katz, "Cavitating Structures at Inception in Turbulent Shear Flow," in *Proceedings of the 10th International Symposium on Cavitation (CAV2018)*, ASME Press, 12 2018.

[22] F. D. Halpern, I. Sfiligoi, M. Kostuk, R. Stefan, and R. E. Waltz, "Simulations of plasmas and fluids using anti-symmetric models," *Journal of Computational Physics*, vol. 445, 2021.

[23] H. Choi and P. Moin, "Grid-point requirements for large eddy simulation: Chapman's estimates revisited," *Physics of fluids*, vol. 24, no. 1, 2012.

[24] Y. Liu, W. Blokland, C. D. Long, B. W. Riemer, M. W. Wendel, and D. E. Winder, "Strain measurement in the spallation target using high-radiation-tolerant fiber sensors," *IEEE Sensors Journal*, vol. 18, no. 9, pp. 3645–3653, 2018.

[25] Y. Liu, D. E. Winder, B. Qi, C. D. Long, and W. Lu, "Upgraded fiber-optic sensor system for dynamic strain measurement in spallation neutron source," *IEEE Sensors Journal*, vol. 21, no. 23, pp. 26772–26784, 2021.

[26] D. A. McClintock, B. W. Riemer, P. D. Ferguson, A. J. Carroll, and M. J. Dayton, "Initial observations of cavitation-induced erosion of liquid metal spallation target vessels at the spallation neutron source," *Journal of Nuclear Materials*, vol. 431, no. 1, pp. 147–159, 2012.

[27] D. S. Viswanath, T. K. Ghosh, D. H. L. Prasad, N. V. K. Dutt, and K. Y. Rani, *Viscosity of liquids: theory, estimation, experiment, and data.* Springer Science & Business Media, 2007.

[28] D. S. Viswanath and B. C. Mathur, "Thermal conductivity of liquid metals and alloys," *Metallurgical and Materials Transactions B*, vol. 3, no. 7, pp. 1769–1772, 1972.

[29] D. Winder, D. McClintock, and D. Bruce, "Cavitation-induced erosion in liquid metal spallation targets – a comparison between a predictive method and measured erosion damage to stainless steel target modules at the spallation neutron source," *Wear*, vol. 450-451, p. 203257, 2020.

[30] P. Kuchhal, R. Kumar, and N. Dass, "Equation of state of liquid metals from sound-velocity measurements," *Physical Review B*, vol. 55, no. 13, pp. 8042–8044, 1997.

[31] S. Ayrinhac, M. Gauthier, L. E. Bove, M. Morand, G. Le Marchand, F. Bergame, J. Philippe, and F. Decremps, "Equation of state of liquid mercury to 520 K and 7 GPa from acoustic velocity measurements," *The Journal of Chemical Physics*, vol. 140, no. 24, 2014.

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

ALMA

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

HDF5

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.

Colleagues mostly, also general community info

Question #2

Suggested Reviewers

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.

No_thank_you.pdf
The attachment is on the following page.

INCITE Committee,

The project "Cavitation inception in turbulent liquid metal" is not interested in utilizing AI testbed resources, Section 9, Question #1 of the application, however there is no option to continue without uploading a file.

Regards,
Mark Kostuk, PI