

# Call for FY 2023 DoD Frontier Project Proposals

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## Introduction

**Purpose:** The Department of Defense (DoD) High Performance Computing Modernization Program (HPCMP) has established DoD Frontier Projects to enable research, development, test and evaluation (RDT&E), and acquisition engineering outcomes that would not be achievable using typically available HPCMP resources.

**Overview:** Please read this section carefully as it details important changes to the Frontier program that have been made in the last two years. In addition, please carefully review the requirements for proposals to ensure that all requirements are met in any submitted proposal. Frontier Projects will continue to pursue outcomes aligned with DoD mission priorities and be supported by multi-year commitments of exceptional amounts of high performance computing (HPC) computational resources.

**Starting in FY 2022, the HPCMP made two significant changes to the Frontier Program.**

- 1. The HPCMP is executing two types of Frontier Projects: Foundational Research and Engineering Frontier Projects and Applied Acquisition and Sustainment Frontier Projects.**
- 2. The HPCMP has implemented a more rigorous review of progress. Projects that are not making adequate progress on initially stated goals may be either reduced in size or terminated.** Additional details are below.

**Foundational Research and Engineering Frontier Projects** follow the guidelines that have been in place since the program started in FY 2014. However, they primarily focus on science and technology (budget activities 6.1, 6.2, and early 6.3). These projects cannot easily be achieved using typically available HPCMP resources, and they are expected to use 100s of millions of core-hours per year and/or 10s of thousands of GPGPU node-hours per year over a 2-4 year period.

**Applied Acquisition and Sustainment Frontier Projects** address DoD design, development, and test and evaluation projects; they focus on programs of record, test and evaluation, and quick response science and technology for urgent operational requirements. This type of project is generally more time-critical, has shorter execution timelines, and is expected to use 10s of millions of core-hours per year and/or thousands of GPGPU-hours over a 1-2 year period. As Frontier Projects, these projects will benefit from higher system priority that shortens timelines with enhanced throughput. Finally, there will continue to be an option to start Applied Acquisition and Sustainment Frontier Projects outside the proposal cycle. The procedures for

this are posted on the HPC website. New Applied Acquisition and Sustainment Frontier Project proposals should be submitted in response to this annual call until this call for proposals expires.

***Eligibility:*** All Frontier Projects must be sponsored by a DoD government scientist/engineer and must use HPCMP resources to enhance mission impact and capability. Principal investigators for Frontier Projects may be scientists or engineers from government, industry, or academia. If the principal investigator is a DoD government scientist/engineer, there is no need to name a separate DoD sponsor.

***Relation to Existing Frontier Projects:*** The HPCMP seeks projects with high DoD mission impact and strong scientific merit. New Frontier Projects should not be duplicative of existing Frontier Projects.

We continue previous years' interest in receiving proposals from key focus areas that have been identified as being of high interest within DoD: (1) hypersonic systems; (2) autonomous systems/artificial intelligence; (3) future vertical lift; (4) electromagnetic development and design, (5) directed-energy systems; and (6) microelectronics. Finally, we continue to be interested in proposals that will be able to leverage the program's investment in shared TS-SCI resources and the new HPCMP systems with significant GPGPU capabilities.

Of the sixteen active Frontier Projects, six projects will complete in FY 2022. The ten projects that will continue to be active in FY 2023 with their corresponding primary computational technology areas (CTAs) are

1. High-Fidelity Modeling and Simulation to Support Army Aviation Acquisition Programs, Andrew Wissink, Army Aviation Development Directorate, AMRDEC (CFD)
2. High-Fidelity Physics-Based Simulation of Kinetic and Directed Energy Weapons Integration Strategies for Future Air Dominance Platforms, Scott Sherer, Air Force Research Laboratory – Air Vehicles (CFD)
3. Terminal Ballistics to Advance Army Modernization Priorities, Robert Doney, Army Research Laboratory (CSM)
4. Whole Atmosphere NEPTUNE, P. Alex Reinecke, Naval Research Laboratory (CWO)
5. Direct Numerical Simulations of Turbulence at Hypervelocity Flight Conditions, Neal Bitter, Office of Naval Research (CFD)
6. M&S for Ground Test and Evaluation, Jason Klepper, Arnold Engineering and Development Center (CFD)
7. Multi-fidelity Design Optimization of Rotating Detonation Engines, Matthew Harvazinski, Air Force Research Laboratory (CFD)
8. HPC Enabled, Digital Transformation for Laser Weapon Systems Development, John Tam, Air Force Research Laboratory (CFD)

9. Large-scale Integrated Simulations of Transient Aerothermodynamics in Gas Turbine Engines, Luis Bravo and Russell Powers, Army Research Laboratory and Naval Air Warfare Center (CFD)
10. Identifying Ultra-high-temperature Ceramics in Multi-Component Chemical Space for Hypersonic Technologies, Stefano Curtarolo, Office of Naval Research (CCM)

The six projects that will complete in FY 2022 are

1. Prediction of Hypersonic Laminar-Turbulent Transition through Direct Numerical Simulation, Jonathan Poggie, Purdue University, sponsored by the Air Force Research Laboratory (CFD)
2. Earth System Prediction Capability, Joe Metzger, Naval Research Laboratory (CWO)
3. Integrated Computational Flight Simulation in Support of the Future Naval Capabilities (FNC) Dynamic Interface Virtual Environment (DIVE) Program, Susan Polsky, Naval Air Warfare Center (CFD)
4. CVN 78 Modeling and Simulation Validation for Full Ship Shock Trial (FSST) Alternative, Timothy McGee, Naval Surface Warfare Center (CSM)
5. CFD for Virginia Sub Sea Warfare (SSW), Susan Brewton, Naval Surface Warfare Center (CFD)
6. Applied Computational Aerodynamics for USAF Weapon Systems, Andrew Lofthouse, Air Force Life Cycle Management Center (CFD)

A summary of all ten projects that will continue into FY 2023 is included in Attachment 1.

**Awards:** Foundational Research and Engineering Frontier Projects may be proposed for up to a four-year duration. Applied Acquisition and Sustainment Frontier Projects may be proposed up to a two-year duration; however, we expect many of these projects will be shorter than two years. Exceptional amounts of HPC computational resources will be provided to each project without regard to any quota based on the proposing Services/Agencies. Support is available from HPCMP assets such as the DoD Supercomputing Resource Centers (DSRCs), User Productivity Enhancement and Training (PET), and the Data Analysis and Assessment Center (DAAC).

**Project Review:** Frontier Projects will be reviewed twice a year by the High Performance Computing Modernization Program Office (HPCMPO). In addition, written quarterly progress reports are required for quarters that do not contain the Annual Project Review or On-Site Visit. The overarching goals of all reviews are to assure projects are on track, delivering mission-relevant impact and to resolve issues that projects are having with HPCMP systems and resources.

- a. **Annual Project Review.** This review will be a formal project review meeting with HPCMP leadership and a technical review panel. As part of this review, HPCMP leadership and the technical review panel will make a progress assessment of each project. Projects that are not making adequate progress on initially stated goals may be

either reduced in size or terminated. The intent is for this to be an in-person meeting with the option to conduct reviews at the Secret collateral level. Project Leaders are expected to attend all project reviews. If travel restrictions are in place, the meeting will be held virtually and content adjusted to meet applicable security rules.

- b. **On-site Visit.** Resource Management leads a small a group that includes Associate Director for Centers representation that visits each project for an in-depth review (normally 2.5 to 4 hours in duration). The primary focus of this review is to discuss significant detail on the technical aspects of the project. Another significant focus is to identify and resolve issues with HPCMP systems, software, and resource.

**Submission:** All Frontier proposals must be submitted through the appropriate Service/Agency High Performance Computing Advisory Panel (HPCAP) principal to the HPCMPO. All proposals must be at the unclassified level. If an exception is needed for a classified submittal, please contact Michael Ausserer, at [michael.f.ausserer.civ@mail.mil](mailto:michael.f.ausserer.civ@mail.mil) or 240-425-9057. Proposals must be received by the HPCMPO by 25 April 2022; however, HPCAP principals have established earlier internal deadlines. The HPCAP points-of-contact and dates for submission of proposals to the Services/Agencies are as follows:

- Air Force: Mr. Bryon Foster ([Bryon.Foster@us.af.mil](mailto:Bryon.Foster@us.af.mil)) and Mr. William Quigley ([William.Quigley.5@us.af.mil](mailto:William.Quigley.5@us.af.mil)). Submit proposals by 21 March 2022.
- Army: Mr. Robert Sheroke ([Robert.M.Sheroke.civ@mail.mil](mailto:Robert.M.Sheroke.civ@mail.mil)), and Mr. Eldred Lopez ([Eldred.I.Lopez.ctr@mail.mil](mailto:Eldred.I.Lopez.ctr@mail.mil)). Submit proposals by 1 April 2022.
- Navy: Ms. Kathy Hollyer ([kathy.hollyer.ctr@navy.mil](mailto:kathy.hollyer.ctr@navy.mil)). Submit proposals by 4 April 2022.
- DTRA: Ms. Jacqueline Bell ([jacqueline.l.bell2.civ@mail.mil](mailto:jacqueline.l.bell2.civ@mail.mil)). Submit proposals by 4 April 2022.
- DARPA: Dr. Nick Lemberos ([nick.lemberos@darpa.mil](mailto:nick.lemberos@darpa.mil)). Submit proposals by 21 March 2022.
- MDA: Mr. Jose Rivera ([jose.rivera.ctr@mda.mil](mailto:jose.rivera.ctr@mda.mil)). Submit proposals by 4 April 2022.

**Evaluation:** Selection will be based on the following two elements:

1. **DoD and warfighter mission impact**
2. **Technical excellence.** A technical review panel will be convened by the HPCMPO. This panel will evaluate proposals using the following criteria:
  - a. Technical merit: Based on the project's goals, solution approach, management approach, and technical quality, what is the value of the computational work to the technical communities to which the project applies?
  - b. Computational merit: How efficiently can the proposed project take advantage of the high performance computing capabilities requested? Is the proposed computational

approach robust and is the software (existing and/or proposed) highly scalable to achieve the desired outcomes?

- c. Potential for progress: Based on the team's qualifications and previous work, does the team have the potential to complete the proposed work?

**Selection:** The HPCMP Director will select the FY 2023 Frontier Projects. Awards will be announced in early August 2022. Selected projects will be provided Frontier allocations starting 1 October 2022.

**Questions:** Contact Mr. Michael Ausserer, HPCMP Associate Director for Resource Management, at [michael.f.ausserer.civ@mail.mil](mailto:michael.f.ausserer.civ@mail.mil) or 240-425-9057.

## Proposal Contents

Frontier Project proposals are limited to 15 pages (single-spaced, standard 12-point font, one-inch margins); it is not necessary that the proposal be 15 pages, provided the required information in each category can be presented in fewer pages. It must be a single Word document, with the exception of the curricula vitae, which must be a separate document. If a Word document cannot be submitted, please contact your Service/Agency and the HPCMPO ([frontier@hpc.mil](mailto:frontier@hpc.mil)) for suitable alternative formats. The cover page, resource request sheets, and any curricula vitae do not count against the 15-page limit. **Proposals must contain the following sections – ordered and numbered as indicated. It is essential that all sections contain the required information in the detail requested.** Suggested lengths for each section are provided.

**Cover Page:** (Length: 1 page maximum, does not count against the 15 page limit; see Attachment 2)

**Project Title:** Provide the title of the project.

**Project Type:** Specify Foundational Research and Engineering or Applied Acquisition and Sustainment.

**Requirements Project Number(s):** Provide the project number(s) (as reflected in the HPCMP requirements database) representing the project requirements on which the Frontier Project proposal is based. A proposal cannot be considered unless its resource requirements are reflected in the HPCMP requirements database. Please contact Tameka Jones at [require@hpc.mil](mailto:require@hpc.mil) for further details.

**Duration:** Specify the expected duration of the project, in years (maximum of four years for Foundational Research and Engineering and two years for Applied Acquisition and Sustainment).

**CTA:** List the primary and associated CTAs that best fit this project.

***Estimated Resources by Year:*** Summarize the total estimated computational requirement on the Project Resource Request sheets by year, in millions of core-hours for traditional CPU requirements and thousands of GPU-hours for GPGPU requirements (see Attachment 3).

***Government Sponsor:*** Provide the Government sponsor's name and contact information, if the principal investigator is not a DoD government scientist/engineer.

***Principal Investigator:*** Provide the Frontier Project's principal investigator's name and contact information. Only one person should be listed, and that person will be the lead for interactions with the HPCMP during the project.

***Key Collaborators:*** Provide a list of organizations or personnel planned to participate in the project.

***Impact:*** Summarize the expected impact of the project to DoD, the warfighter, and the technical community.

***Technical Goals and Approach:*** Summarize the technical objectives of the project and the planned computational approach.

***Major Applications Software:*** List major applications software that will be used.

***Technical & Computational Challenges:*** Summarize anticipated challenges for the project and the planned computational approach.

## Technical Proposal

Include the following topics in the proposal narrative:

**Introduction:** Introduce the project in broad terms. Include a general discussion of ongoing related work in both your organization and the scientific, technology, and/or testing community. (Length: approximately ½ to 1 page)

**DoD Impact:** Clearly state the DoD mission impact of the project and any current and future programs of record it will support. State the advantage to be gained by utilizing HPC capability. (Length: approximately ½ to 1 page)

**Technical Approach:** Clearly state the technical goals of the project and discuss the science, technology, and/or engineering activities that are required to meet these goals. Provide a plan for achieving these goals. Discuss technical challenges that will likely be encountered during the course of the project and how they will be overcome. (Length: approximately 3-6 pages)

**Schedule and Anticipated Accomplishments:** State clearly the duration of the project and provide a schedule in tabular form with estimated milestones and anticipated accomplishments for each year. **This is a key component of the proposal because it will be used to measure progress in the annual project review.** (Length: approximately ½ to 1 page)

**Computational Approach:** Describe the computational methodology and algorithms, and estimate the size of the problem with as many supporting details as possible. Discuss the relationship between early year developments and later year accomplishments. Discuss applicable software efficiency on scalable systems by stating the performance as a function of the degree of parallelism. Show evidence that the software provides sufficient foundation to scale to the problem size needed to achieve the goals of the project and/or discuss software developments that will be required as a part of the project. Scalability information, including a graph of application performance for a typical test case versus the number of cores and/or GPUs, should be included. **It is also particularly important that application codes are either fully developed or ready for use by each proposed project, or specific plans to reach that state of readiness are detailed in the proposal.** Discuss optimal computational architectures relative to available HPCMP resources. Discuss the computational challenges that will likely be encountered during the course of the project, how they will be overcome, and how this project will add to the computational state-of-the-art in this technical area. **Detailed justification must be provided for the level of computational resources required.** (Length: approximately 2-4 pages)

**Progress to Date:** Discuss preparatory work in the proposed technical area in this section. Elaborate on any HPC resources previously used by this project and/or efforts leading up to this

proposed project. Discuss what work remains and how a Frontier Project can facilitate achieving the proposed work. (Length: approximately ½ to 2 pages)

**Key Personnel:** Identify the key personnel who will work on this project and summarize the background and qualifications of each participant, including each participant's projected level of effort. Provide an estimate of the size of the group that will perform this work, including an estimate of the percentage of time each team member will contribute to the project. Also include a discussion of possible incorporation of HPCMP team members into the project team. (Length: approximately 1-2 pages)

**Required Computational Resources and Justification:** Outline the computational resources required to accomplish this project in terms of total core-hours and/or GPU-hours on HPCMP systems for all years of the project. **Provide requirements based on specific, current HPCMP systems for FY 2023 and FY 2024.** These early year requirements must be definitive and reasonably accurate. **For the out-years, an estimate of the required number of core-hours and/or GPU-hours can either be stated on current HPCMP systems or on a generic system architecture expected to be available. A list of current HPCMP systems is available at <https://centers.hpc.mil>.** Justification for the required level of computational resources can be provided by documenting known run times on the same or similar architectures as proposed for the project and scaling those to address the project's goals. Include a discussion of any specialized memory, storage, networking, and/or software requirements. (Length: approximately 1-3 pages)

**Computational Summary Sheet:** Provide estimates of computational resources required to accomplish the proposed project. A completed DoD Frontier Project Resource Request (see Attachment 3; not part of 15-page limit) for each year of the proposed project is required. The form is divided into three sections:

- Section I: Specify the applicable year and enter the principal investigator information.
- Section II: There are two tables in Section II. The first table facilitates outlining suites of systems at various locations that can address the project's requirements. Proposals may present multiple scenarios (combinations of platforms and locations). The second table, which contains computational processor, memory, and data archive storage requirements, must be completed once for each year of the project.
- Section III: Enter the computational project titles and project numbers (as reflected in the HPCMP requirements database) associated with the project. Please contact Tameka Jones at [require@hpc.mil](mailto:require@hpc.mil) if you need assistance with this.

**Curricula Vitae:** Provide a *curriculum vita* (including a list of relevant publications) for each of the key personnel. (**in a separate document**; not part of 15-page limit)

# Attachment 1

## Summary of Existing Frontier Projects

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### **High-Fidelity Modeling and Simulation to Support Army Aviation Acquisition Programs (Andrew Wissink, Army Aviation Development Directorate, AMRDEC)**

The goal of this project is to integrate the CREATE-AV Helios and Kestrel high-fidelity modeling and simulation tools into Future Vertical Lift acquisitions of interest to Army Aviation to demonstrate the impact of these tools for the acquisition of major defense systems by reducing cost, development time, and risk. The project performs high-fidelity multi-disciplinary computational modeling and simulation for the Future Attack and Reconnaissance Aircraft (FARA), Future Long Range Attack Aircraft (FLRAA), and Future Unmanned Air Systems (FUAS) acquisition programs in Future Vertical Lift (FVL), in order to characterize performance, loads, vibration, noise, and safety to inform decision teams. Frontier resources enable high quality computational analysis of these configurations with a high-resolution digital model before the expensive manufacturing and flight test phase of the acquisition. Because FUAS has a longer-term development cycle (scheduled DoD insertion FY27), the project initially focuses on newly envisioned applications of the current Gray Eagle UAS configuration presently used by the Army.

### **High-Fidelity Physics-Based Simulation of Kinetic and Directed Energy Weapons Integration Strategies for Future Air Dominance Platforms (Scott Sherer, Air Force Research Laboratory)**

The goals of this project include development of robust flow-control options for integration of directed and kinetic energy weapon systems on future air dominance platforms, and demonstration of selected options on a representative maneuvering vehicle. To accomplish these goals, high-fidelity, unsteady CFD using primarily DDES to design and evaluate flow control options are being used. Novel script-based grid generation are used to quickly develop and simulate new geometries. Overset grid techniques are used to incorporate selected concepts onto vehicles and dynamic, moving grid simulations are being performed.

### **Whole Atmosphere NEPTUNE (P. Alex Reinecke, Naval Research Laboratory)**

The major goal of this project is to use the NEPTUNE deep atmospheric model to develop and validate a high-resolution global numerical weather prediction system to support IOC and replace the existing Navy global NWP system. In addition, the project is developing and testing a unique, whole atmosphere forecasting capability, extending from the Earth's surface to 500 km height with the goal of predicting thermospheric disturbances at unprecedented spatial and temporal scales. The work supports existing ONR, NRL, and DARPA projects by performing numerical experiments with NEPTUNE of the whole atmosphere. Hindcasts for 30-60 day periods at increasing horizontal

resolution are being done to validate new physical parameterizations, data assimilation techniques, and ensemble predictions in NEPTUNE. The project is designed to support the U.S. Navy's capabilities to characterize the current and future state of the battlespace environment in order to ensure battlespace dominance in the 21st century.

### **Terminal Ballistics to Advance Army Modernization Priorities (Robert Doney, Army Research Laboratory)**

The goal of this project is to advance survivability and lethality capabilities in support of Army modernization priorities. A variety of codes are being used to perform continuum and mesoscale simulations to optimize armor and lethal mechanisms as well as evaluate and mature new protection concepts. Atomistic, microscale, and mesoscale simulations are being used to capture microstructural effects on energetic materials for improved prediction of detonative response as well as material discovery. This work is critical to advancing DoD capability in three of the U.S. Army's six Modernization Priorities: Long Range Precision Fires, Next Generation Combat Vehicle, and Soldier Lethality.

### **Direct Numerical Simulations of Turbulence at Hypervelocity Flight Conditions (Neal Bitter, Johns Hopkins Applied Physics Laboratory, sponsored by the Office of Naval Research)**

The goal of this project is to address the basic science of hypervelocity turbulent flow and the application of turbulence models for real flight vehicles. It uses direct numerical simulations (DNS) to identify and address deficiencies in existing turbulence models for aero-heating prediction, a key risk area for hypersonic vehicle design. DNS methods are being executed at flight relevant conditions for both unclassified and classified vehicle designs. These predictions are used to evaluate performance of Reynolds Averaged Navier Stokes (RANS) models. The results of these analyses will establish credibility and quantify uncertainty of RANS models for aeroheating and aerodynamic analyses to reduce uncertainty in predictions of these important quantities, which are critical to design of hypersonic vehicles for DoD programs.

### **M&S for Ground Test and Evaluation (Jason Klepper, Arnold Engineering Development Center)**

The goal of this project is to apply timely modeling and simulation (M&S) support to increasingly complex test requirements, including broader regions of test envelopes and for more tests at AEDC. It uses M&S to plan tests, to compare M&S and test results, to form a digital twin of the system under test, and to resolve test anomalies. Various CFD applications are used throughout the acquisition lifecycle and throughout the T&E process at AEDC. During pre-test, CFD simulations aid in test planning, predicting results, test article/test cell interaction, test matrix reduction, and determining where to place the test article and instruments. During tests, on-line CFD is provided to understand incoming data and plan the course of the test as it progresses. After test, CFD simulations guide analysis, especially if the test data does not match the simulations or pre-test predictions within an acceptable margin of error. Overall, application of M&S early in the acquisition lifecycle saves time and thus funds for the program by establishing an authoritative digital twin of the system, reducing test matrices, and identifying issues earlier than they would be if caught during ground or flight test.

## **Multi-fidelity Design Optimization of Rotating Detonation Engines (Matthew Harvazinski, Air Force Research Laboratory)**

The goal of this project is to deliver improved rotating detonation engine (RDE) operability limits and performance through multi-fidelity design optimization using simulations with various CFD applications. These simulations are being used for two specific areas of design optimization. Injector optimization will yield injectors that promote mixing and yield a higher percentage of combustion in detonation over deflagration. Nozzle optimization will result in better-conditioned flow with higher thrust. The overall effort will enable four 6.3 RDE programs: liquid fuel ram RDE for Mach 3 internal carriage air to ground munitions, solid fuel ram RDE for air to air munitions, RDEs for turbine engine augmentation (afterburner), and RDE Freejet test program.

## **HPC Enabled, Digital Transformation for Laser Weapon Systems Development (John Tam, Air Force Research Laboratory)**

The goal of this project is to utilize HPC to enable high physical fidelity End-to-End Model (EtEM) simulation to buy-down technical risks in laser weapon systems (LWS) technology development. Specifically, the project will focus on weapon lethality, digitally connect LWS solutions across TRLs, accelerate the transition process, and reduce costs. The EtEM package is being used to model air-based laser weapon system scenarios including: source modeling, beam control, adaptive optics, aero-optics, atmospheric propagation, scene generation, and damage modeling and lethality. Individual high fidelity models for laser sources and turbulence are providing data used by EtEM. The overall result will provide significant technological advantage for space domain awareness, improve laser weapon system transition efforts by simulating solution strategies for technical risks to system performance, and connect those solutions to weapon lethality in the context of engagement simulation.

## **Large-scale Integrated Simulations of Transient Aerothermodynamics in Gas Turbine Engines (Luis Bravo, Army Research Laboratory; and Russell Powers, Naval Air Warfare Center)**

The goal of this project is to advance the state-of-the-art in Digital Engineering tools by developing a massively parallel LES design framework for integrated simulations of unsteady engine analysis. The project plans to demonstrate applicability by conducting multi-component analyses of OEM engines at a sweep of design and off-design conditions. The thrust areas to be investigated are 1) onset of transients and performance in unsteady inlet and compressor integrated models, 2) onset of combustor dynamics using jet fuel chemistry and high temperature strongly-coupled turbine fluid structure interactions, and 3) advancing industry standard integrated simulations in gasturbine engine extreme environments. The project will culminate with a sweep of integrated simulations of the PWAPU engine (62T-46C12) operating at off-design conditions and demonstration of improved performance. Rigorous uncertainty quantification and machine learning will be key for real-time and accurate engine design tools. Success of this project will lead to engines with increased performance, efficiency, and reliability at a much lower development cost in shorter timelines; incorporate these tools into a high-fidelity Digital Twin engine model that will enable real time engine health awareness and reduced lifecycle cost; and mitigate particle ingestion that will increase engine service life and mission readiness for operations in austere environments.

## Identifying Ultra-high-temperature Ceramics in Multi-component Chemical Space for Hypersonic Technologies (Stefano Curtarolo, Duke University, sponsored by Office of Naval Research)

The goal of this project is to identify multi-component disordered entropic reciprocal ultra-high-temperature ceramics (ER-UHTCs) that form high-entropy single phases with high-hardness values, train machine-learned interatomic potentials for multi-component ceramics, and develop a materials similarity search tool to provide collections of materials with similar properties. The Automatic FLOW Framework for Materials Discovery (AFLOW) is being used to simulate materials and calculate their properties with density functional theory. Structural, electronic, thermodynamic, and thermo-mechanical properties are automatically analyzed, and descriptors are used to identify compositions that are likely to form disordered materials with high-hardness. An active machine learning workflow is being implemented with a training feedback loop to refine the search space towards compositions with superior-hardness. Promising candidates will be experimentally synthesized, and the corresponding Vickers hardness will be measured. The project will lead to suitable high-temperature and high-pressure materials to withstand the extreme-environment conditions for DoD applications, such as reusable hypersonic vehicles, inside rocket engines, and friction stir welding.

# Attachment 2

## FY 2023 DoD Frontier Project Proposal Cover Page

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## FY2023 DoD FRONTIER PROJECT PROPOSAL COVER PAGE

<b>Project Background</b>		
Project Title:		
<b>Project Type: either “Foundational Research and Engineering” or “Applied Acquisition and Sustainment”</b>		
Requirements Project Number(s):	CTA(s):	Project Duration (in years):
Estimated Core-hours and/or GPU-hours by year: FY23-	FY24-	FY25-      FY26-
<b>Government Sponsor</b>		
Name:	E-mail Address:	
Organization:	Phone Number:	
<b>Principal Investigator (may be the same as Government Sponsor)</b>		
Name:	E-mail Address:	
Organization:	Phone Number:	
<b>Key Collaborators</b>		
Names & roles:		
<b>Impact</b> (Specify the impact of the project’s outcomes to DoD, the warfighter, and the technical community)		
<b>Technical Goals</b>		
<b>Technical Approach</b>		
<b>Major Applications Software</b> (e.g., ANSYS CFD)		
<b>Technical &amp; Computational Challenges</b>		
<b>Cover material limited to one page – row heights may be adjusted to suit</b>		

# Attachment 3

## DoD Frontier Project Resource Request

**Submit a complete copy of the information in attachment 3 for each year.**

# DoD Frontier Project Resource Request

## **Section I: General Information**

Project Number and Title: \_\_\_\_\_ Project Year: \_\_\_\_\_

Principal Investigator:

Name: \_\_\_\_\_ Service/Agency: \_\_\_\_\_ Organization: \_\_\_\_\_

Address, City, State, and Zip Code: \_\_\_\_\_

\_\_\_\_\_

E-mail Address: \_\_\_\_\_

Phone: \_\_\_\_\_

## **Section II: Overall Project Resource Requirements**

Platform(s)	Location (DSRC)		CPU Resources (core-hours)	GPU Resources (GPU-hours)
	First Choice	Second Choice	Request	Minimum Acceptable

Platform(s)	Typical Number of Processors	Maximum Number of Processors	Typical Job Memory (GB)	Maximum Job Memory (GB)	Total Data Archive Storage Requirements (TB)

Total Expected Working Storage Requirements (in TB): \_\_\_\_\_

Annual Expected Archival Storage Requirements (per year in TB): \_\_\_\_\_

### **Section III: Requirements Project Information**

#### **HPCMP Requirements Database Information:**

Project Title from HPCMP Requirements Database: \_\_\_\_\_

Project Number from HPCMP Requirement Database: \_\_\_\_\_