# Call for FY 2019 DoD Frontier Project Proposals

## Introduction

***Purpose***: The Department of Defense (DoD) High Performance Computing Modernization Program (HPCMP) established DoD Frontier Projects to enable the exploration of research, development, test and evaluation (RDT&E) and acquisition engineering outcomes that would not be achievable using typically available HPCMP resources. Frontier Projects pursue outcomes aligned with DoD mission priorities and are supported by multi-year commitments of exceptional amounts of high performance computing (HPC) computational resources (i.e., 100s of millions of core-hours per year).

***Eligibility:*** The Department of Defense (DoD) High Performance Computing Modernization Program (HPCMP) established DoD Frontier Projects to enable the exploration of research, development, test and evaluation (RDT&E) and acquisition engineering outcomes that would not be achievable using typically available HPCMP resources. Frontier Projects pursue outcomes aligned with DoD mission priorities and are supported by multi-year commitments of exceptional amounts of high performance computing (HPC) computational resources (i.e., 100s of millions of core-hours per year).

***Relation to Existing Frontier Projects:*** The HPCMP seeks projects with high DoD impact, and encourages applicants to propose work that is not duplicative of existing Frontier Projects. Of the twelve active Frontier Projects, four projects will complete in FY2018. The eight projects that will be active in FY2019 with their corresponding computational technology areas (CTAs), https://www.hpc.mil/index.php/technology-areas/computational-tech-areas, are

1. Petascale High Fidelity Simulation of Atomization and Spray/Wall Interactions at High Temperature, Luis Bravo, Army Research Laboratory (CFD)
2. Advancing DoD Modeling and Prediction Capabilities in the Arctic, Wieslaw Maslowski, Naval Postgraduate School (CWO)
3. Development of Multi-scale Models for Materials Design, Mark Gordon, Iowa State University, sponsored by the Air Force Research Laboratory (CCM)
4. Terminal Ballistics for Lethality and Protection Sciences, Robert Doney, Army Research Laboratory (CSM, CCM)
5. HPC Modeling and Simulation to Support DoD Rotorcraft Acquisition Programs, Andrew Wissink, Army Aviation Development Directorate, AMRDEC (CFD)
6. Validation of Turbulence and Turbulent Combustion Models for Air Force Propulsion Systems, Venkateswaran Sankaran, Air Force Research Laboratory (CFD)

7. Navy Electromagnetic Railgun, Joel Mejeur, Naval Surface Warfare Center (CSM, CFD, CEA)
8. Prediction of Hypersonic Laminar-Turbulent Transition through Direct Numerical Simulation, Jonathan Poggie, Purdue University, sponsored by the Air Force Research Laboratory (CFD)

The four projects that will complete in FY 2018 are:

1. Multi-scale Interactions in Stratified Turbulence, Stephen de Bruyn Kops, University of Massachusetts, sponsored by the Office of Naval Research (CFD)
2. Unsteady Pressure and Heating Environment on High-Speed Vehicles with Responding Structures, Ryan Gosse, Air Force Research Laboratory (CFD)
3. Dynamics and Properties of High-Speed Turbulent Reacting Flows, Alexei Poludnenko, Texas A&M University, sponsored by the Air Force Research Laboratory (CFD)
4. Earth System Prediction Capability, Joe Metzger, Naval Research Laboratory (CWO)

A summary of all twelve projects is included in Attachment 1.

***Awards:*** A Frontier Project may be proposed for a two-to-five-year duration. 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, Technology Transfer and Training (PETTT), and the Data Analysis and Assessment Center (DAAC).

***Project Review:*** Frontier Projects will be formally reviewed twice a year by the High Performance Computing Modernization Program Office (HPCMPO); a formal project review meeting with all Frontier Project Principal Investigators (PIs) present, and an in-person, on-site visit to each project site focusing on an in-depth review of the technical aspects of the project. Written quarterly progress reports are required for quarters that do not contain either of the project review meetings. Projects are expected to have frequent interaction with DSRC and PETTT support personnel.

***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. Proposals must be received by the HPCMPO by 27 April 2018; 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. Darrell Phillipson (darrell.phillipson@us.af.mil) and Mr. Bryon Foster (Bryon.Foster@us.af.mil). Submit proposals by 2 April 2018.
- Army: Mr. Robert Sheroke (Robert.M.Sheroke.civ@mail.mil), and Mr. Eldred Lopez (Eldred.I.Lopez.ctr@mail.mil). Submit proposals by 16 April 2018.

- Navy: Ms. Kathy Hollyer (kathy.hollyer.ctr@navy.mil). Submit proposals by 16 April 2018.
- DTRA: Ms. Jacqueline Bell (jacqueline.l.bell2.civ@mail.mil). Submit proposals by 16 April 2018.
- DARPA: Dr. Nick Lemberos (nick.lemberos@darpa.mil). Submit proposals by 2 April 2018.
- MDA: Ms. Jennifer Phifer (jennifer.phifer@mda.mil). Submit proposals by 16 April 2018.

***Evaluation:*** A technical review panel convened by the HPCMPO will evaluate proposals using the following criteria:

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

Technical review panel evaluations will be used in conjunction with Service/Agency and OSD mission impact scores to formulate a recommendation for project selection by the HPCMP Director. Awards will be announced in early August 2018.

***Questions:*** Contact Mr. Michael Ausserer, HPCMP Associate Director for Resource Management, michael.ausserer@us.af.mil, 937-255-6614.

## Proposal Contents

Frontier Project proposals are limited to 15 pages (single-spaced, standard 12-point font, one-inch margins) and must be a single Word document. If a Word document cannot be submitted, please contact your Service/Agency and the HPCMPO (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. Suggested lengths for each section are provided.

### Cover Page: (Length: 1 page maximum; see Attachment 2)

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

***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 Cathy McDonald at require@hpc.mil for further details.

***CTA:*** List the primary and associated CTAs that best fit this project (see https://www.hpc.mil/index.php/technology-areas/computational-tech-areas).

***Duration:*** Specify the expected duration of the project, in years.

***Estimated Core-hours by Year:*** Summarize the total estimated computational requirement described on the Project Resource Request sheets by year, in millions of core-hours.

***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.

***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.

***DoD Impact:*** Summarize the projected DoD impact.

***Community Impact:*** Summarize the projected impact on the scientific and engineering community.

## 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 exploiting 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)

***Timeline 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. (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, should be included. Discuss optimal computational architectures relative to available HPCMP resources. Discuss the computational challenges that will likely be encountered during the course of the project and how they will be overcome. (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, and 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 on specific HPCMP systems for FY 2019 and FY 2020. These early year requirements should be definitive and reasonably accurate. For the out-years, an estimated number of core-hours on a generic system architecture expected to be available during the out-years may be stated. 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 Cathy McDonald at 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. (Not part of 15-page limit)

# Attachment 1
# Summary of Existing Frontier Projects

### Multi-scale Interactions in Stratified Turbulence (Stephen de Bruyn Kops, University of Massachusetts, sponsored by the Office of Naval Research)

The technical goal of this project is to generate research simulations at Reynolds numbers that are relevant to engineering problems in the ocean or atmosphere. In addition, turbulence subjected to stabilizing buoyancy forces will be modeled so that fast simulations can accurately predict the performance of vehicles, sensors, and weapons in the deep ocean and atmosphere. Very large direct numerical simulations of simple flow configurations will be performed in order to understand the dynamics of stratified turbulence.

### Unsteady Pressure and Heating Environment on High-Speed Vehicles with Responding Structures (Ryan Gosse, Air Force Research Laboratory)

This Frontier Project seeks to determine the fully-coupled high fidelity fluid-thermal-structural response of high-speed vehicles at full scale that resolves all relevant physics of the fluid and structure domains. Specific coupled computational fluid dynamics (CFD) and structural application codes will be optimized, scaled, and tested for their ability to address important flow features in boundary layers. These techniques will be applied to hypersonic Air Force strike weapons to impact and control costs for test programs of these vehicles.

### Dynamics and Properties of High-Speed Turbulent Reacting Flows: From a Jet Engine to an Exploding Star (Alexei Poludnenko, sponsored by the Air Force Research Laboratory)

The uniform grid and static mesh refinement code Athena-RFX will be developed and tested by incorporating detailed kinetic reaction models for light hydrocarbon fuels and thermal/barodiffusion. A systematic study will be performed of turbulent flames in $H_2$-air, $H_2$-CO, and light hydrocarbon fuels for a broad range of turbulent intensities, system sizes, and equivalence ratios, both in the pre-mixed and non-pre-mixed regimes. The results will advance the fundamental understanding of high-speed, turbulent, reacting flows that will impact a number of systems of interest to DoD, including scramjet engines for hypersonic flight and detonation-based engines for efficient onboard power generation and propulsion.

## Petascale High Fidelity Simulation of Atomization and Spray/Wall Interactions at High Temperature and Pressure Conditions (Luis Bravo, Army Research Laboratory)

This project seeks to perform extensive three-dimensional simulations of the mixture formation process in direct injection engines, with a particular emphasis on the spray atomization process and spray/wall interactions. An understanding of the complex physics involved in these processes from these simulations will be used to enhance current engineering models for predicting these processes. The outcomes of this project will include both new high-fidelity direct Navier-Stokes simulation codes as well as the detailed understanding of these processes, which can then be used to improve several Army direct injection engine technologies by increasing power density and engine efficiency, while reducing battlefield signatures.

## Advancing DoD Modeling and Prediction Capabilities in the Arctic (Wieslaw Maslowski, Naval Postgraduate School)

This Frontier Project has the overall goal of advancing the understanding of and resolving processes and feedbacks controlling the operation of the Arctic region's ocean and sea ice systems, reduce uncertainty in modeling those systems, and improve the prediction of Arctic sea ice and climate using state-of-the-art modeling applications. The results of this work will aid Arctic stewardship and U.S. interests in line with DoD and national strategies for the Arctic region and provide accurate projections of regional climate change.

## Development of Multi-scale Models for Material Design (Mark Gordon, Iowa State University, sponsored by the Air Force Office of Scientific Research)

This Frontier Project's goal is the development and application of a multi-scale method that seamlessly integrates electronic structure theory methods, parameter-free coarse-graining methods, and molecular dynamics/Monte Carlo simulation methods to provide accurate and efficient predictions of bulk properties of advanced materials, without the need for empirically fitted parameters. The new multiscale simulation methods will be implemented in the widely-used GAMESS code, thus making these new capabilities available to a broad user base in government, industry, and academia. The methodologies will be applied to accurate computation of the properties of ionic liquids, which, as potential new propellants, may have significant impacts to DoD, including (a) reliable and cost effective access to space, (b) improved satellite maneuverability and increased on-orbit lifetime, and (c) reduction of environmental and toxicological hazards and improved safety associated with propellant storage and handling.

## Terminal Ballistics for Lethality and Protection Sciences (Robert Doney, Army Research Laboratory)

This Frontier Project seeks to advance the state-of-the-art in terminal ballistics by focusing on three themes: rigorous uncertainty quantification of ballistic events, understanding human response to ballistic loading, and breakthrough capability for materials modeling. Each area requires multi-scale continuum and mesoscale modeling capability. Successful investigation of these three themes will further develop the quality of shock physics codes which provide critical modeling capability to enable significant DoD advances in armor, lethality, and hypervelocity impact.

## HPC Modeling and Simulation to Support DoD Rotorcraft Acquisition Programs (Andrew Wissink, Army Aviation Development Directorate, AMRDEC)

The overall goal of this Frontier Project is to demonstrate for the first time that high-fidelity modeling and simulation tools such as the CREATE-AV™ Helios flow solver can actually have a significant impact in the acquisition of major defense systems by reducing their cost, development time, and risk. This project will perform high-fidelity multi-disciplinary computational modeling and simulation for the JMR-TD and CH-47 DoD acquisition program vehicles. These computations will be used to evaluate performance, loads, vibration, noise, and safety in the proposed new designs prior to and during their upcoming flight tests.

## Validation of Turbulence and Turbulent Combustion Models for Air Force Propulsion Systems (Venkateswaran Sankaran, Air Force Research Laboratory)

The goal of this Frontier Project is the development, validation, and application of advanced turbulence and turbulent combustion models designed specifically for Air Force propulsion applications, including gas turbines, scramjets, and rockets. Reacting direct numerical simulations (DNS) and large eddy simulations (LES) coupled with existing and new turbulence, combustion, and turbulent combustion modes will be evaluated using a hierarchy of unit physics, canonical and grand challenge problems in gas turbines, augmentors, rockets, and scramjets.

### Earth System Prediction Capability (Joe Metzger, Naval Research Laboratory)

The overall goal of this Frontier Project is to perform the R&D necessary to produce the Navy's contribution to the national Earth System Prediction Capability (ESPC). Specifically, this will be our first operational global long-range coupled forecast system for the atmosphere, ocean, sea ice, and waves that extends beyond a week to a month or more. The core components of this ESPC system are the Navy's current global prediction models for seven-day forecasts. Data assimilation will also initially use the Navy's current separate atmosphere and ocean products loosely coupled via the coupled forecast model as a first approximation. We use multi-year re-analyses and re-forecasts to test and understand the system. The target for IOC is a 30-day ensemble forecast, but much of our testing will be with 45- or 60-day re-forecasts since we expect to extend the range for FOC.

### Navy Electromagnetic Railgun (Joel Mejeur, Naval Surface Warfare Center)

This Frontier Project will support basic science and applied studies on development of the electromagnetic railgun launcher technologies through the end of ONR's initial phase in the technology development of these systems. This project will expand understanding of the complex behavior within the molten interface between the rail and armature, thus increasing the understanding of armature and launcher dynamics of a railgun and assisting with detailed analysis of the launcher performance. The project builds on an initial three-year Frontier Project in this same area which addressed and overcame many of the multi-disciplinary computational and technical challenges of successfully modeling and simulating electromagnetic railguns, and the current project extends the effort to include both analysis of the in-bore flow fields and their impact on shot performance and detailed analysis of electromagnetic fields with the projectile.

### Prediction of Hypersonic Laminar-Turbulent Transition through Direct Numerical Simulation (Jonathan Poggie, Purdue University, sponsored by Air Force Research Laboratory)

The objective of this project is to improve the prediction of hypersonic laminar-turbulent transition, and consequently to improve the prediction of heating rates in hypersonic flight. It will predict acoustic noise and transition in conventional hypersonic wind tunnels to make these facilities more useful for vehicle design. Direct numerical simulation (DNS) of hypersonic boundary layer receptivity will be performed to predict the acoustic noise spectrum radiated from turbulent boundary layers on wind tunnel walls and examine the effects on boundary layer transition of disturbances introduced from the free-stream and at the tunnel wall. With this new understanding of the effects of tunnel noise, conventional hypersonic wind tunnels will be useful for testing hypersonic vehicles in spite of this noise.  This may would save the DoD the cost of a new hypersonic quiet facility, an investment of at least $20M with 5-10 years of development. The proposed work will impact several DoD programs in hypersonics, including the High-Speed Strike Weapon (HSSW).

# Attachment 2
# FY 2019 DoD Frontier Project Proposal Cover Page

## FY2018 DoD FRONTIER PROJECT PROPOSAL COVER PAGE

| | | |
|---|---|---|
| **Project Background** | | |
| Project Title: | | |
| Requirements Project Number(s): | CTA(s): | Project Duration (in years): |
| Estimated Core-hours by year: FY19- FY20- FY21- FY22- FY23- | | |
| **Government Sponsor** | | |
| Name: | Email Address: | |
| Organization: | Phone Number: | |
| **Principal Investigator (may be the same as Government Sponsor)** | | |
| Name: | Email Address: | |
| Organization: | Phone Number: | |
| **Key Collaborators** | | |
| Name & role: | | |
| **Technical Goals** | | |
| | | |
| **Technical Approach** | | |
| | | |
| **Major Applications Software** (e.g., ANSYS CFD) | | |
| | | |
| **Technical & Computational Challenges** | | |
| | | |
| **DoD Impact** (Specify the impact of the project's outcomes to DoD) | | |
| | | |
| **Community Impact** (Describe the project's impact on the scientific and/or engineering community) | | |
| | | |
| **Cover material limited to one page – row heights may be adjusted to suit** | | |

# Attachment 3

# DoD Frontier Project Resource Request

## 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) | |
|---|---|---|---|---|
| | First Choice | Second Choice | Request | Minimum Acceptable |
| | | | | |
| | | | | |
| | | | | |
| | | | | |
| | | | | |
| | | | | |

***Note: If needed, insert multiple copies of the table above.***

| 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:______________________________