

FY 2022 Frontier Projects

The HPCMP established DoD Frontier Projects in FY13 to enable the exploration of RDT&E and acquisition engineering outcomes that would not be achievable using typically available HPCMP resources. These projects are DoD high-impact RDT&E computational efforts that are selected through a rigorous evaluation process that includes both OSD and Service/Agency mission-relevance and technical excellence. The Frontier Project portfolio represents the Program's most computationally-demanding, resource-intensive set of projects that require sustained and extensive assistance from the entire HPCMP ecosystem (DSRCs, user support, software development, PET, and networking) to fully succeed. For FY22 there are fourteen active Frontier Projects following the completion of one project at the end of FY21, and the start of five new projects in FY22. A steady-state of 10-15 Frontier Projects is expected to be maintained for the foreseeable future. The Frontier portfolio is expected to continue to utilize 25% to 30% of HPCMP total computational resources and, thus, represents a considerable resource investment on potential breakthrough concepts.

One of the new FY22 Frontier Projects is of a new type of Frontier Project, Applied Acquisition and Sustainment. FY22 is the first year that includes two types of Frontier Projects: Foundational Research and Engineering Frontier Projects and Applied Acquisition and Sustainment Frontier Projects:

- (1) Foundational Research and Engineering Frontier Projects** follow the guidelines that have been in place since the program started in FY 2013. They primarily focus on science and technology work (budget activities 6.1, 6.2, and early 6.3). These projects cannot easily be achievable 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.
- (2) 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 node-hours over a 1-2 year period. As Frontier Projects these projects benefit from higher system priority that shortens timelines with enhanced throughput.

The Frontier Project portfolio spans the entire RDT&E and acquisition engineering spectrum, from basic research through direct support to acquisition programs at the decision-making stage. Many of these projects are interdisciplinary in nature crossing the boundaries between two or more technical disciplines. DoD organizations executing these projects include each Service's primary research laboratories and basic research granting agencies, as well as other Service laboratories. Principal investigators are from government and academia. Over 100 scientists and engineers are active Frontier users on the HPCMP systems. In FY21, Frontier Projects used approximately 1.5 billion core-hours on HPCMP systems. Projects included leading-edge research in combustion, chemistry, and turbulence; development of weather and ocean models to support DoD operations;

Army and Navy rotorcraft acquisition programs; Army armor development; and direct support to test and evaluation programs.

Each FY22 Frontier Project is summarized below.

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 simulations (DNS) of hypersonic boundary layer receptivity are 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 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 work impacts several DoD programs in hypersonics, including the High-Speed Strike Weapon (HSSW).

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 the 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 use the Navy's current separate atmosphere and ocean products loosely coupled via the coupled forecast model as a first approximation. Multi-year re-analyses and re-forecasts are used to test and understand the system. The target for IOC is a 30-day ensemble forecast, but much of the testing will be with 45- or 60-day re-forecasts because the range for FOC is expected to be extended.

Integrated Computational Flight Simulation in Support of the Future Naval Capabilities Dynamic Interface Virtual Environment Program (Susan Polsky, Naval Air Warfare Center – Aircraft Division)

This Frontier Project's goal is to predict the limits of flight envelopes for rotorcraft landing on ships. The project uses CFD coupled with Manned Flight Simulator aircraft flight dynamics

models to accurately predict the non-linear aerodynamics affecting helicopter performance and pilot workload due to coupling between atmospheric winds/ship airwake, dynamic control surface motion (as controlled by the aircraft flight control laws and autonomous pilot inputs), and aircraft motion relative to the ship. These models are being further developed, tested, and validated against wind tunnel and flight test data.

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.

CVN 78 Modeling and Simulation Validation for Full Ship Shock Trial (FSST) Alternative (Brian Lang, Naval Surface Warfare Center – Carderock Division)

NAVSEA has been tasked by SECNAV's office with performing M&S in advance of the summer 2020 USS GERALD R. FORD (CVN 78) Full Ship Shock Trial (FSST) in an effort to validate the Navy Enhanced Sierra Mechanics (NESM) software using blind, pre-trial predictions to support an FSST alternative. This task has completed NESM simulations for all 3 planned FSST shots prior to the 2021 FSST. The NESM software is being validated against data that has been recorded during the next FSST, which has been conducted against the CVN 78 in the summer of FY21. One hundred fifty shock response sensors were installed on CVN 78 specifically for this effort, which provided an ample data set against which to validate NESM for predicting equipment dynamic inputs under shock loading.

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)

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 – Aircraft Division)

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 Curatolo, 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.