National Aeronautics and
Space Administration

HECC Annual Report FY22

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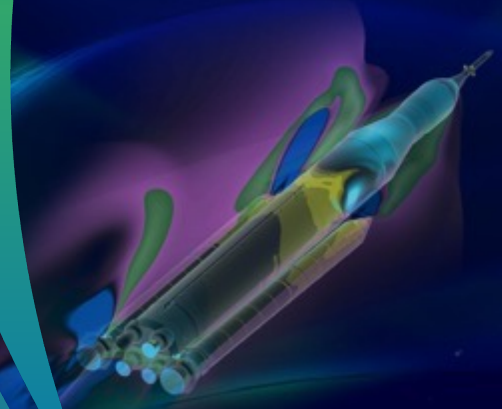
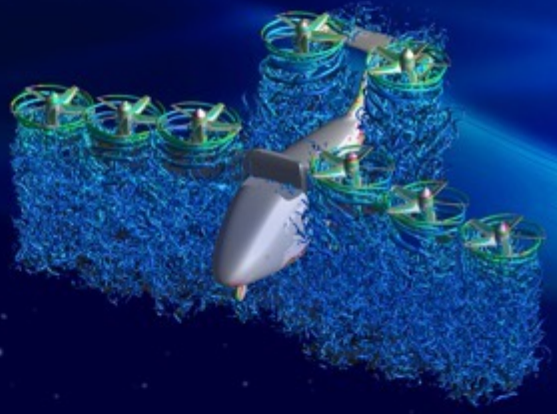
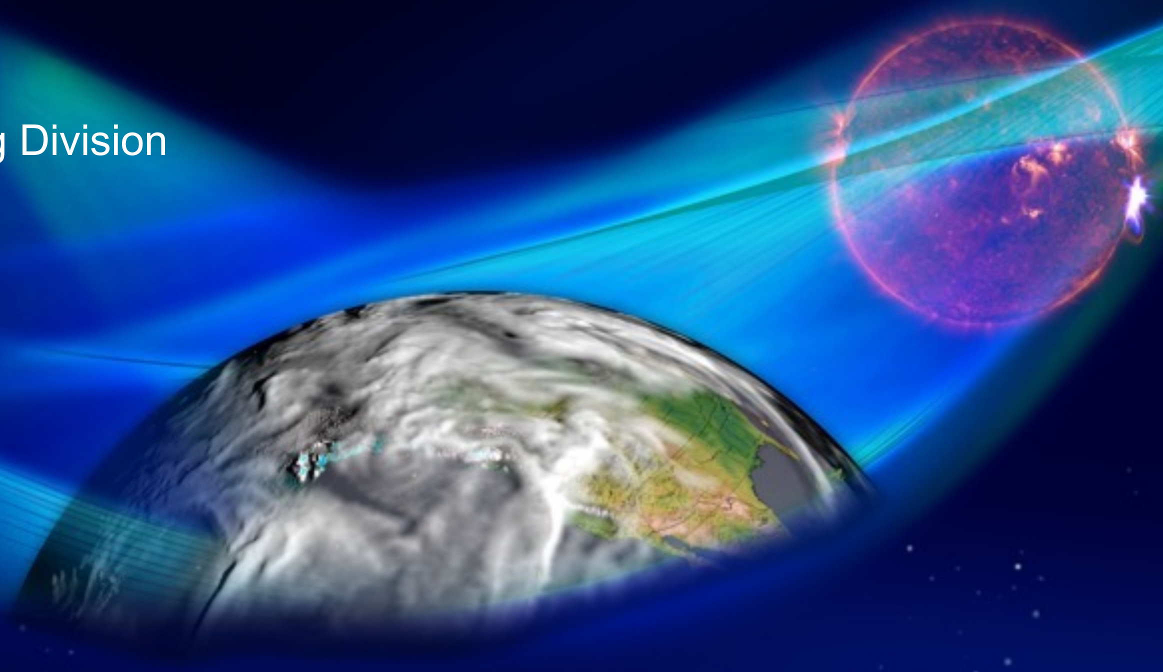
NASA Advanced Supercomputing Division

May 24, 2023







High-End Computing Capability: FY22 Annual Report

- The High-End Computing Capability (HECC) project, established in 2008, has a broad vision that spans all NASA mission areas:

  NASA's HECC resources are relied on as an essential and pervasive partner by the breadth of agency science, engineering, and technology activities, enabling rapid advances in insight and dramatically enhancing mission achievements.

- Toward that vision, in Fiscal Year 2022, HECC delivered nearly 140 million Standard Billing Units (SBUs*)—essential to the success of 840 unique projects supporting ARMD, STMD, SOMD, ESDMD, HEOMD, NESC, and SMD.
- This year HECC also celebrated several major successes:
  - **Aitken is now NASA's most powerful supercomputer** with a theoretical peak performance of 13.12 petaflops.
  - **HECC's cloud infrastructure team** successfully transitioned science teams to run computational fluid dynamics (CFD) simulations on Amazon Web Services cloud resources.
  - **New Data Science and Data Portal features** improve the ability to run machine learning applications and make it easier for scientists and engineers to share datasets with both NASA and external collaborators.
  - **New DDN filesystems and an improved InfiniBand network** increase storage capacity and improve overall Lustre storage system reliability and performance for HECC users.

**1 SBU equals 1 hour of a Pleiades Broadwell 28-core node.*

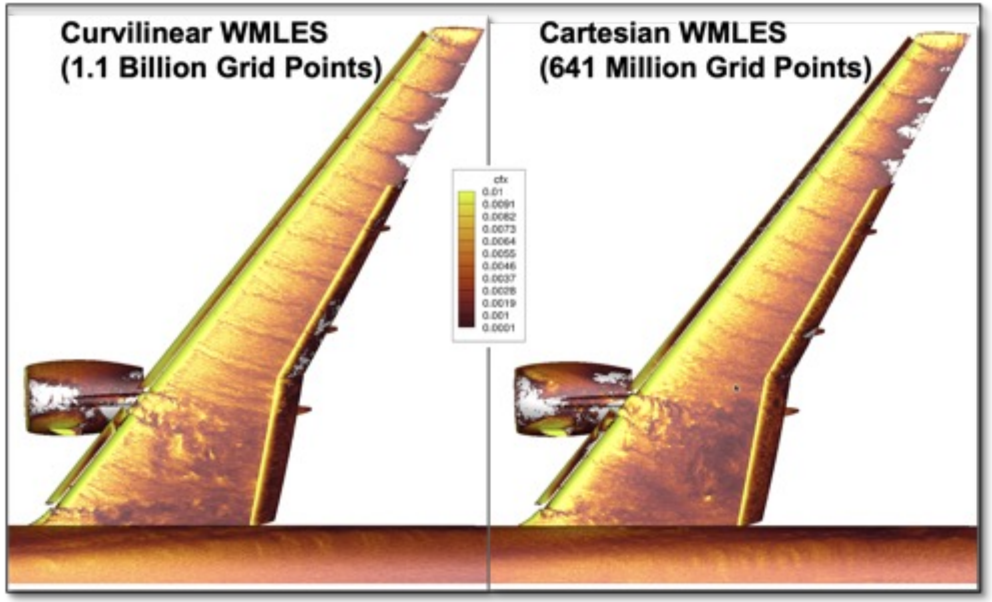
Modular Supercomputing Facility: Sustainability in Action

- The Modular Supercomputing Facility (MSF) continues to exemplify the NASA High-End Computing Program's commitment to conservation of environmental resources through HECC operations, yielding substantial savings in energy and water usage compared to traditional facilities.
  - The MSF's Aitken and Electra supercomputers produce industry-leading annual Water Usage Effectiveness (WUE) ratings of 0.21 Liters per kilowatt hour (L/kWh). In comparison, the Department of Energy reports an average data center WUE of 1.8 L/ kWh.
  - Electra and Aitken each had a Power Usage Effectiveness (PUE) of 1.05. PUE is an established metric for computer center power efficiency. In comparison, the reported average PUE for data centers around the world is 1.8; and the PUE for all of NASA is 1.48.
- NASA's most powerful and sustainable supercomputer, Aitken was expanded to 13.12 petaflops in 2022, increasing the system's theoretical peak performance by 49% since 2021.
- HECC experts improved the resilience and maintainability of the InfiniBand network connected to Aitken, and devised a new power measurement method for Aitken's AMD Rome nodes to identify and correct load imbalances of users' codes on the system and improve efficiency of resource usage.
- With HECC's innovative modular supercomputing model, additional modules can be connected together as needed to accommodate the agency's ever-increasing demand for computing resources.

The Aitken supercomputer is housed in a single module of NASA's Modular Supercomputing Facility (MSF), which resides at NASA Ames on a one-acre site with the infrastructure to support 16 modules. The agency plans to install a second module in 2024. In this artist's rendition, the MSF is shown at its full potential buildout to 16 modules.
Marco Librero, NASA Ames

Cloud Computing through HECC AWS Resources

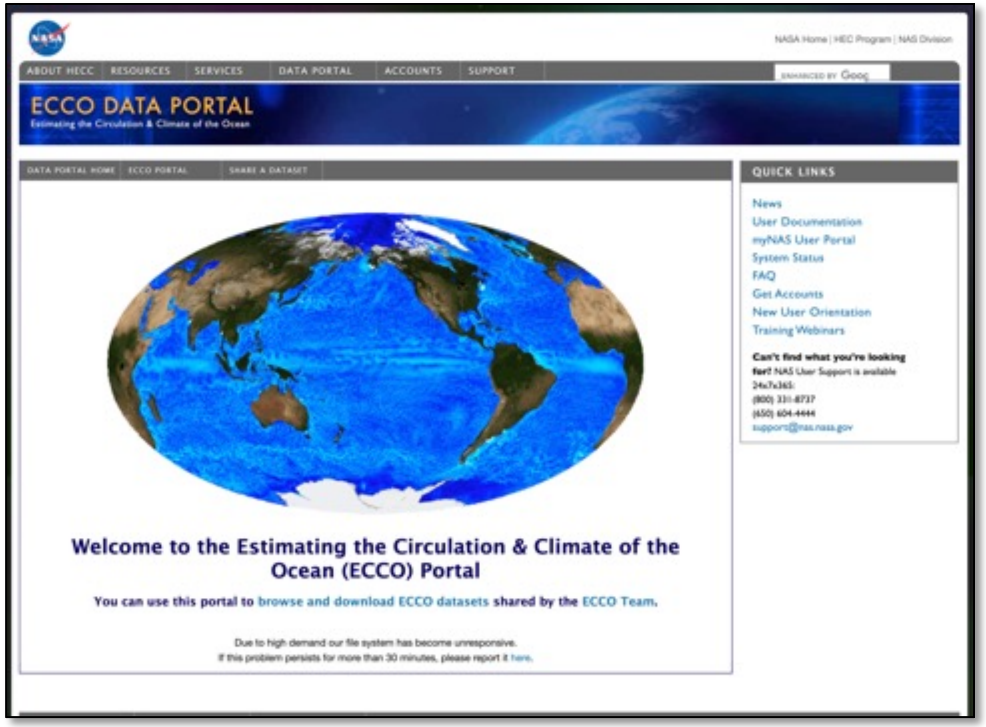
- During FY22, HECC staff worked with several science teams to develop a flow from Amazon Web Services (AWS) cloud resources to compute systems within the HECC enclave for compute-intensive components of their work.
- The Launch, Ascent, and Vehicle Aerodynamics (LAVA) team at the NASA Advanced Supercomputing Division used the HECC cloud and supercomputing resources to carry out Wall-Modeled Large-Eddy Simulation (WMLES) studies of the High-Lift Common Research Model. The team found that the per-node performance and interconnect of AWS resources are comparable to or even better than HECC systems.
  - Their work utilized up to 160 c5n-type AWS nodes with each queue wait time never exceeding five minutes.
  - Visualization and post-processing can both be completed in the cloud, eliminating the need for large data transfers and dedicated post-processing workstations.
  - However, when only looking at the costs of the nodes(s), on-demand cloud resources are approximately 5–8 times more expensive than in-house HECC resources. Resource managers/allocators should look at the full costs to determine if cloud is the optimal solution for their problem.
- HECC technical staff also prototyped a PBS scheduler-integrated data caching mechanism that will allow researchers to use large, diverse datasets from cloud infrastructures more efficiently with on-prem systems.



LAVA prediction of instantaneous surface skin friction for two WMLES cases utilizing AWS and in-house resources. Availability of on-demand HECC cloud resources enables important NASA applications to be performed in a timely matter in order to meet critical milestones.
Gaetan Kenway, NASA Ames

New Data Science Features and Data Portal Improvements

- In order to better serve HECC’s expanding Data Portal user base, several key features were added in FY22, including:
  - A highly requested method to easily download datasets in bulk through a custom ”wget” command enables recursive downloads of all files and subdirectories using common syntax.
  - A “force” command allows dataset owners to publish dataset changes themselves, automating the sharing of files and directories without affecting the source data on HECC filesystems.
  - A private dataset feature allows owners to share with specific collaborators, including non-NASA affiliates.
- HECC’s Big Data team launched the THREDDS Server, which allows users to download subsets of the scientific data available on the Data Portal. THREDDS allows external users to browse available datasets through a web interface and download files using a variety of remote access protocols. The new server will also allow Web Coverage Service clients to specify a subset of a gridded dataset, gather metadata information, and/or visualize the extracted data through common software packages.
- The HECC Data Science team used the Dask library to speed up the data-generation process for the Spectral Water Inversion Processor and Emulator (SWIPE) tool, which is used by the Biospheric Science team at NASA Ames to generate synthetic bio-optical datasets of alga particles for modeling water quality. This reduced the time needed to create synthetic data and generate a spectral library on one Broadwell node from two hours to 18.5 minutes.



More than five petabytes of data are available in the HECC Data Portals, with external users downloading more than 250 terabytes in 2022. Data Portal and Data Science staff are continually improving features to make it easier to share datasets for both owners and recipients. As this capability evolves, new enhancements continue to be driven by requests from the HECC user base.

HECC Storage Augmentation and Pathfinding Systems

Storage Augmentation

- In FY22, Lustre filesystem capacity was increased by approximately 75%—from 62.7 to 110 petabytes—with the deployment of three new Data Direct Networks (DDN) filesystems. In addition to expanding storage capacity, deployment of the new systems increases overall Lustre storage system reliability and improves performance for HECC users. An enhanced InfiniBand network also improves access to all filesystems.
- HECC user home filesystems were also expanded with new RAID hardware with storage capacity of 300 gigabytes per disk—four times larger than the previous RAID equipment.

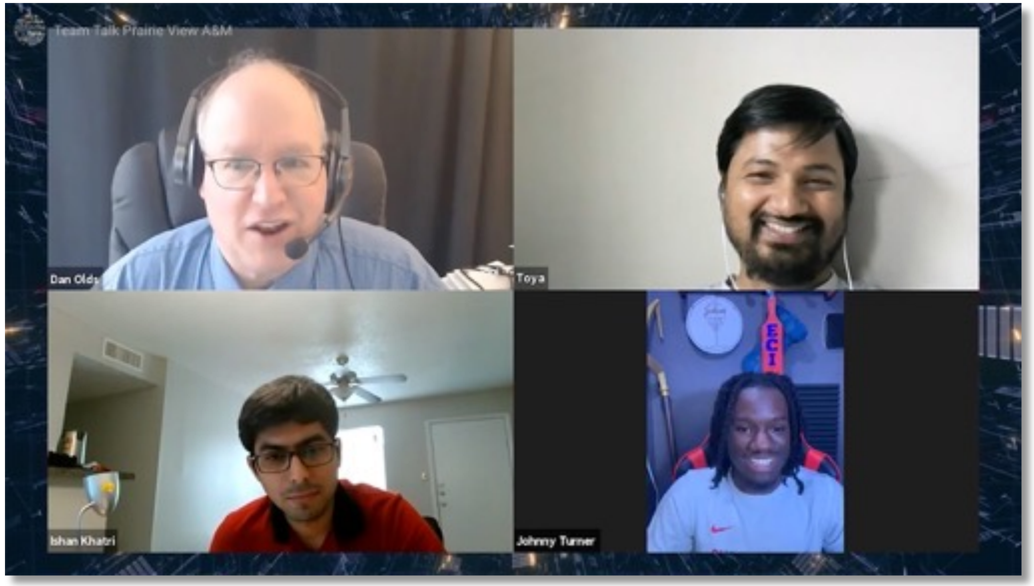
Pathfinding Systems

- To best meet NASA's future physics-based modeling and simulation requirements, HECC is investigating alternate architectures that could shape the project's processor architecture roadmap in the medium term.
  - Vector1 and Vector2: Two specialized compute nodes with NEC Vector Engines will help explore ways to address bottlenecks between memory and processors.
  - AMD Instinct MI100 GPU System: Testing showed encouraging performance; HECC experts recommended additional investigation with AMD's new MI200 GPU. GPU-accelerated systems have the potential to lower the cost of computing for a significant portion of HECC's workload.

HECC's new RAID storage has the capacity to store four times the amount of scientific data than the previous RAID hardware. The migration of home filesystems to the newer hardware was done transparently while the filesystems were in production, with no impact to users.
Don Story, NASA Ames

Fostering STEM Education: Student Cluster Competition

- In alignment with NASA's strategic goal to to foster STEM education and engage and support Minority Serving Institutions, a team of HECC supercomputing experts hosted a NASA segment of the second annual Winter Classic Invitational Student Cluster Competition, mentoring students from minority institutions to gain experience with high-performance computing.
- During a week-long round of competition, the HECC experts provided hands-on instruction to twelve student teams of undergraduate and graduate students from six Historically Black Colleges and Universities and four Hispanic Serving Institutions.
- Using three subsets of the NAS Parallel Benchmarks (NPB), the student teams ran 3,480 computational jobs on Pleiades, with the challenge to help evaluate the performance of parallel supercomputers that run simulations for designing safe and efficient airplanes and spacecraft. The students ran multi-zone versions of the NPB and tested the effectiveness of multi-level and hybrid parallelization paradigms and tools.
- The competition gave a diverse group of student's firsthand practice in developing skills to prepare them for positions in HPC and gave NASA a source for attracting the next generation of HPC professionals.
- After the competition, several students expressed great interest in working at NASA—and one student came onboard as a summer intern working in the NASA Advanced Supercomputing Division.



Students from Prairie View A&M University won the top prize in the 2022 Winter Classic Invitational Student Cluster Competition held March 6–12, 2022. Clockwise from top right: Toya Acharya, Johnny Turner, Ishan Khatri; Aaron Brown (not pictured). Dan Olds, Chief Research Officer, Intersect60 Research, is pictured at top left.
Image courtesy of Intersect360 Research

HECC Achievements Showcased at SC22, Agency Awards

HECC Teams Return to In-Person NASA Exhibit at SC22

- HECC staff planned and produced NASA's booth at SC22, the International Conference for High-Performance Computing, Networking, Storage, and Analysis, held November 13–18, 2022 in Dallas, TX, interfacing with more than 11,000 attendees during the agency's in-person return to the annual conference.
- The NASA@SC22 website features 36 science and engineering projects enabled by HECC and NCCS supercomputers and supported by visualization, optimization, and machine learning experts. The projects represent teams from four NASA centers, plus university and industry collaborators.

HECC Staff Recognized with Agency and Center Honor Awards

- HECC staff were honored with several awards during FY22, including:
  - NASA Exceptional Public Achievement Medal (Steve Heistand).
  - NASA Ames Safety Award (Blaise Hartman, Chris Tanner).
  - NESC Administrative Excellence Honor Award (Blaise Hartman).
  - NASA Group Achievement Awards (Network Team; COVID-19 HPC Consortium Support Group; Essential Onsite Response Team; and Support Group for Mission Assurance System).

The SC22 exhibit support team and presenters representing all mission directorates provided thousands of conference attendees with a memorable NASA experience. The annual supercomputing conference provides a highly visible public platform to showcase NASA science and engineering missions supported by the agency's high-performance computing resources. ***James Kling, NASA Goddard***

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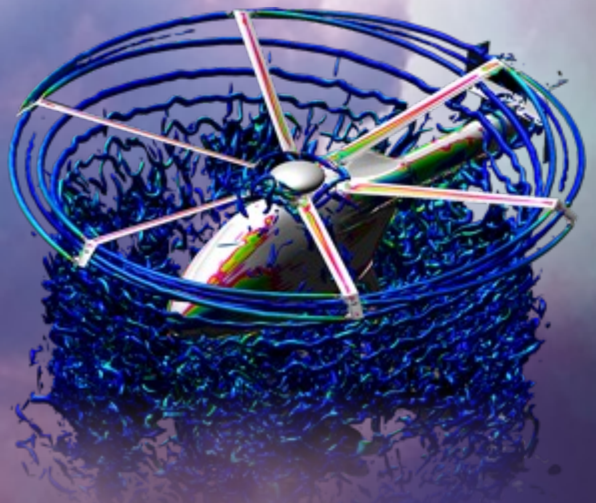
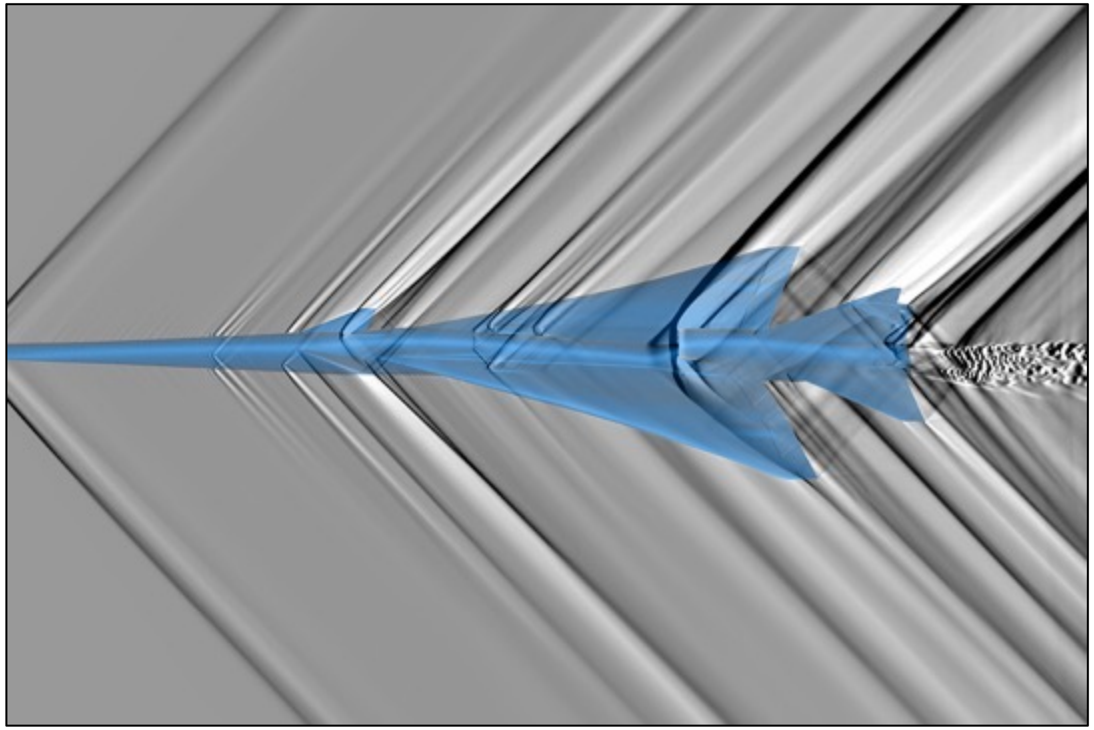


HECC Annual Report FY22

Aeronautics Research Mission Directorate

HECC FY22: Aeronautics Research Mission Directorate

- Many of ARMD’s innovative modeling and simulation breakthroughs, critical to NASA’s collaboration with aircraft industry partners and attaining the agency’s vision for advancing sustainable aviation technology and safety, rely on HECC supercomputing resources and technical expertise.
- The investment in HECC systems and services grew to 166 ARMD projects in FY22, providing scientists and engineers with nearly 40 million SBUs* to meet their program objectives.
- Ten representative projects are highlighted, with a focus on advancing computational capabilities to develop, evaluate, validate, and test next-generation concepts, including the X-57 Maxwell, the hybrid electric transonic truss-braced wing, and multi-rotor urban air mobility (UAM) vehicles. These projects contributed to several program level reviews and milestones and produced more than 30 publications in FY22.
- HECC’s collaboration with ARMD will continue to return innovations and solutions to solve future aviation challenges, meet the growing demand for Urban Air Mobility, and provide more fuel-efficient aircraft and other technologies to reduce the effect of air transportation on the environment.

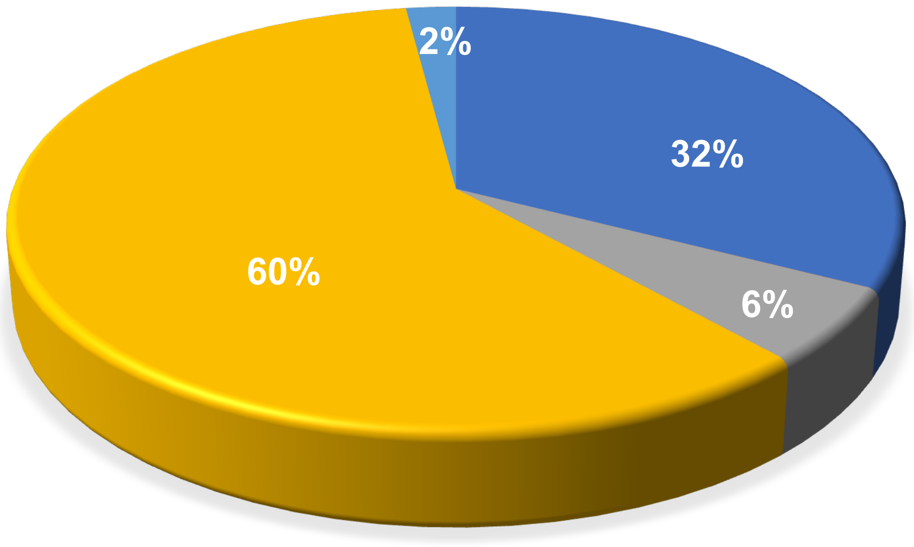


**1 SBU equals 1 hour of a Pleiades Broadwell 28-core node.*

HECC FY22: Aeronautics Research Mission Directorate

- **Total Usage: 38,142,387 SBUs**
  - **Number of Projects:** 166
  - **Average CPU Range:** 4,097 – 8,192 CPUs
  - **Average Expansion Factor:** 2.53
  - **Agency Reserve:** 8,405,394 SBUs
  - **Share:** 30,961,745 SBUs
  - **Usage as Percent of Share:** 123%
  - **Usage as Percent of Share + Agency Reserve:** 97%
- **By ARMD Program**
  - **Transformative Concepts:** 22,753,322
  - **Advanced Air Vehicles Program:** 12,387,056
  - **Integrated Aviation Systems Program Office:** 2,208,968
  - **Aeronautics Evaluation and Test Capabilities:** 788,609
  - **Airspace Operations and Safety Program:** 4,433

ARMD FY22 Usage



**1 SBU equals 1 hour of a Pleiades Broadwell 28-core node.*

Investigating CFD-Based Predictions for Wind Tunnel Tests

Summary

- In support of the Aeroscience Evaluation and Test Capability Office, researchers in the Computational Aerosciences Branch at NASA Ames used the resources provided by HECC to compare computational fluid dynamics (CFD) predictions on a simple wing-body aircraft configuration in the Langley Unitary Plan Wind Tunnel. Their goal was to determine whether CFD can accurately predict the aerodynamics of the model and the flow field in the test evaluation.

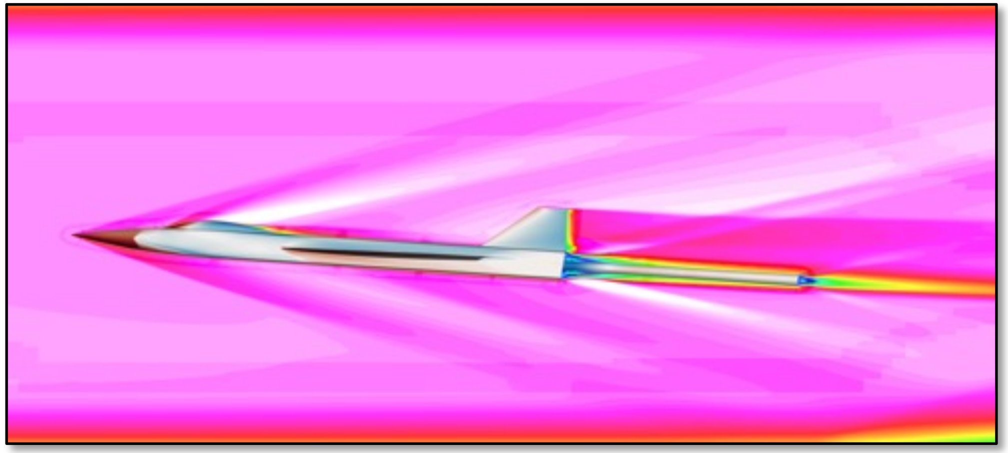
Key Results

- Using the LAVA and Kestral CFD codes, the team generated flow simulations across 140 test conditions, including different Mach numbers, with and without a model in the wind tunnel's test section. They compared experimental and CFD measurements and found that over 60% of the LAVA results were within experimental uncertainty. The main source of discrepancy was uncertainty in the model geometry (the model had to be reconstructed from old design drawings, laser scans, and physical measurements) and the accuracy of the empty-test section CFD predictions.

Role of HECC

- Access to the resources provided by HECC provided the team with the computing required to test modeling capabilities and run databases of scientifically relevant size within a feasible timeframe for the project.

BENEFIT: Understanding the capability of CFD to simulate the aerodynamics of test articles in NASA wind tunnels can provide a basis for better decisions about future investments in the facilities, in addition to learning more about the flow in the wind tunnels and what measurements will benefit further development of CFD tools.



"Without HECC resources, the complex and time-consuming simulations of wind-tunnel flow fields would be impossible. The flow visualization tools provided by HECC experts help us gain essential insight into the computed flow fields, enabling greater under-standing of complex or unexpected wind-tunnel tests."
— James Ross, NASA Ames

High Fidelity Hybrid Electric TTBW Simulation Capability

Summary

- The unconventional configuration of the Transonic Truss-Braced Wing (TTBW) concept design leads to complex flow phenomena such as transonic buffet, separated flow, and a turbulent wake. Using HECC resources, NASA Ames researchers ran Unsteady Reynolds Averaged Navier-Stokes (URANS) and Hybrid RANS Large Eddy Simulations (HRLES) to evaluate the accuracy and efficiency of both approaches to simulating the TTBW.

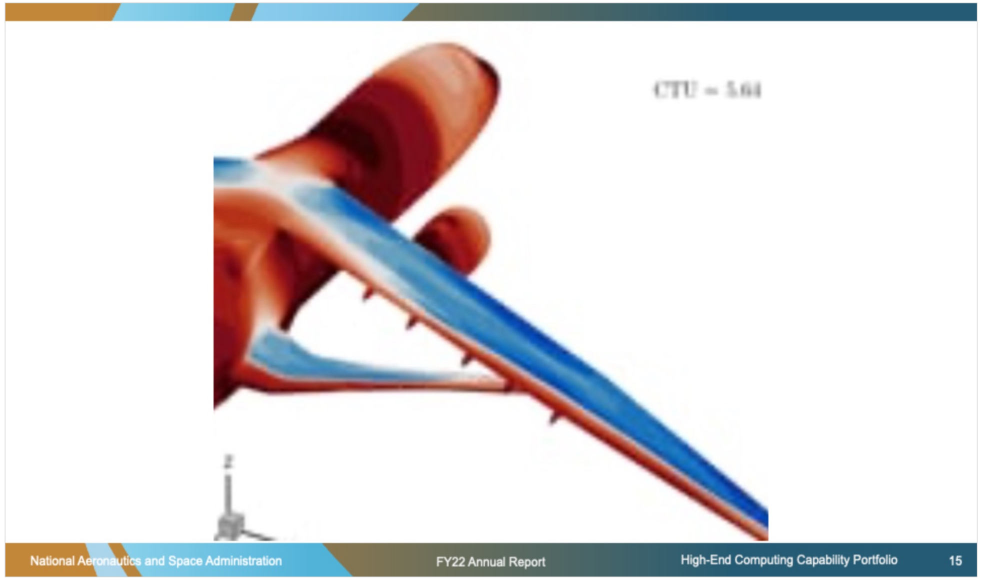
Key Results

- Results indicate that URANS appears to perform better than HRLES in predicting buffet onset at a lower computational cost; however, its accuracy tends to decrease for certain conditions, and scale-resolving methods are necessary to conduct further vehicle analysis. This work will reduce future cost by improving HRLES simulations and determining the levels of uncertainty for all methods going forward. Overall, the team gained a deeper understanding about the TTBW concept and shared those findings with the TTBW project and other NASA teams.

Role of HECC

- Scale-resolving simulations are computationally expensive due to the small timestep size and grid cell sizes needed to resolve the unsteady turbulent flow. Each simulation ran across 50 AMD Rome processors for several days on HECC's Aitken supercomputer.

BENEFIT: In the pursuit of a more fuel-efficient narrowbody commercial aircraft design, NASA invests a considerable amount of resources toward research into transonic truss-braced wing (TTBW) concepts. By improving understanding of this type of aircraft, this work will help the agency develop a flight demonstrator.



"HECC resources made it possible to run Hybrid RANS-LES simulations within a short turnaround time, enabling quick decision-making and accelerating the development of simulation best practices."

— Oliver Browne, NASA Ames

Developing High-Lift Computational Tools for FUN3D

Summary

- In support of NASA's Transformational Tools and Technologies (TTT) Technical Challenge, researchers at NASA Langley are developing and evaluating eddy-resolving methods for high-lift flows using HECC supercomputing resources. The team has developed wall-modeled large-eddy simulation (WMLES) and delayed detached-eddy simulation (DDES) tools for both finite-volume and finite-element discretizations in Langley's FUN3D software.

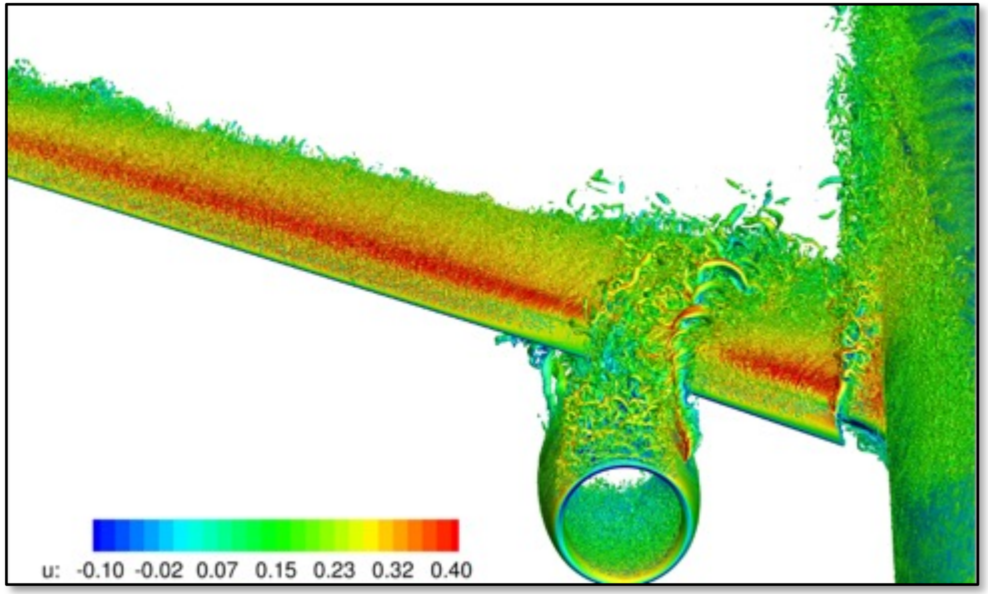
Key Results

- The team continues to expand simulation capabilities within FUN3D. Comparing their simulations with other, similar algorithms, they demonstrated that their results are of similar accuracy and computational efficiency. This critical work for the TTT Technical Challenge is providing tools for simulating flows at maximum lift, and is also part of a cross-agency effort to evaluate other methodologies.

Role of HECC

- Resources available through HECC were vital to the success of this effort, where many simulations required as many as 20,000 CPU cores and 108 GPUs. HECC provides the only resources for the agency suitable for meeting the goals of the project, and the support staff was very helpful and always responsive to any questions.

BENEFIT: The results of this work and the tools developed will provide the agency and aeronautics community with the resources to design and predict the performance of future high-lift aircraft configurations, and also aid in evaluating other methodologies, thereby improving the agency's computational capabilities.



"Our milestones for this project would not have been possible to achieve without HECC resources. Our finite-volume discretization simulations used many GPUs and CPUs." — *William Anderson, NASA Langley*

Evaluating Large-Eddy Simulation for Aeronautics Models

Summary

- As part of the agency's efforts to improve computational fluid dynamics (CFD) capabilities, researchers at NASA Langley performed wall-resolved and wall-modeled large-eddy simulations (WRLES/WMLES) on HECC systems to assess state-of-the-art models for predicting turbulent separation—a phenomena that has been challenging to predict using steady-state Reynolds-Averaged Navier-Stokes (RANS) models.

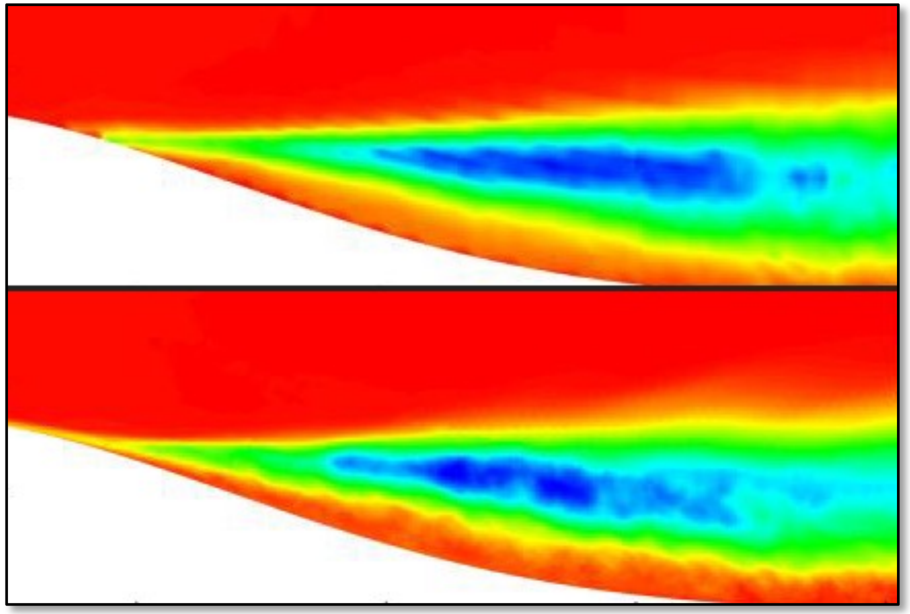
Key Results

- The Langley team proposed a new dynamic, nonlinear subgrid scale model that better captured turbulent smooth-body separation when compared to current linear models. They found that using WRLES on a grid 16 times coarser than earlier high-fidelity simulations gave excellent predictions, but was computationally expensive for the 3D experimental configuration.
- Using insights from high-fidelity simulations, they refined the "internal layer" in the accelerating region of the flow, which produced turbulent separation for WMLES and yielded excellent predictions compared to experiments.

Role of HECC

- This work uses computational grids between 200–600 million cells, which require 2,000–10,000 cores to solve over 2–3 weeks. The team's high-fidelity numerical simulations performed on HECC systems utilized more than ten billion nodes during this period.

BENEFIT: WMLES has shown promising success for complex aeronautic flows such as predicting stall, yet best practices still need to be established. The insights gathered from this work will be useful for related and future agency projects dealing with turbulent flow separation.



"HECC resources enable us to routinely perform parametric sweeps of our computations and simulate higher Reynolds numbers and larger computational domains, making our results more relevant to practical applications."
— *Prahladh Iyer, NASA Langley*

High-Fidelity Simulations of the X-57 Maxwell Concept

Summary

- The NASA Langley X-57 Computational Fluid Dynamics group, in collaboration with industry and researchers at other NASA centers, generated CFD solutions on HECC resources to create an aerodynamic database for a piloted simulator and airworthiness assessments prior to the first flight of the all-electric X-57 Maxwell airplane. The X-57 will use a distributed electric propulsion system to increase lift at takeoff and landing conditions and will cruise efficiently at 150 knots true airspeed, at an altitude of 8,000 feet.

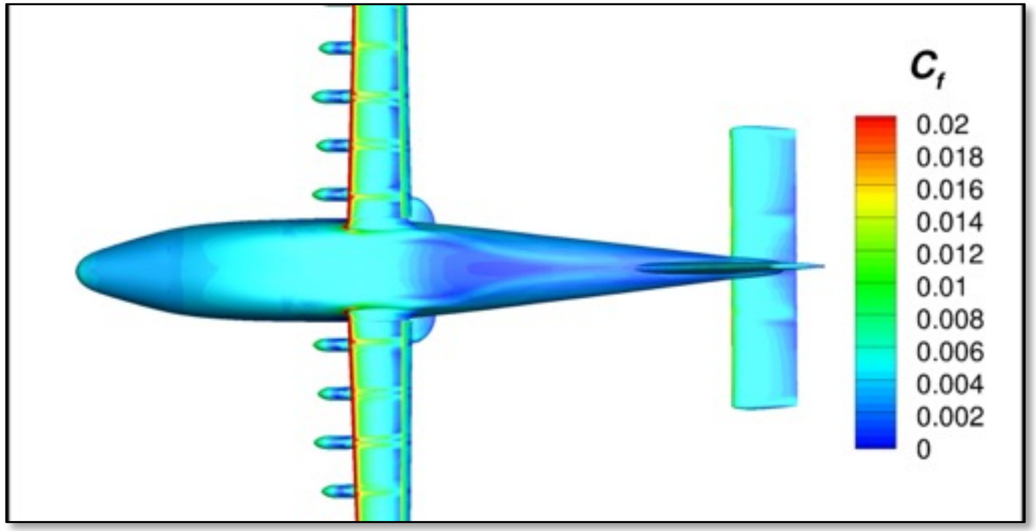
Key Results

- The Langley team updated results for a higher fidelity fuselage geometry and completed an initial study of the impacts of detached-eddy simulations (DES) on high-lift performance. Improved results from USM3D, USM3D-ME, and Kestrel codes reduced differences in unpowered lift between the codes for the 10° flap configuration. Initial studies with the higher-order DES had a large effect on lift for the 30° flap configuration, compared to previous results with Reynolds-Averaged Navier-Stokes equations, indicating further analyses are needed.

Role of HECC

- HECC support for maintaining the Kestrel code on the Pleiades supercomputer is highly beneficial to the work done at Langley. The team used Pleiades for the high-fidelity time-accurate solutions they researched this year. Over 405,000 SBU hours were used on meshes up to 275 million cells, which required up to 900 CPUs per solution.

BENEFIT: With little experimental data for the all-electric X-57 Maxwell, this project provides critical data for a piloted simulator, airworthiness assessments, and safety analyses prior to the plane's first flight. All computational improvements or data repeats contribute to building confidence in the X-57 piloted simulator.



"HECC resources allowed for an improved X-57 piloted simulator by providing the resources necessary to investigate code and mesh improvements with repeat simulations. HECC provided the critical code support needed for Kestrel."

— Karen Deere, NASA Langley

Predicting Proprotor-Wing Interaction Aerodynamics

Summary

- Researchers at the University of California, Davis ran high-fidelity computational fluid dynamics (CFD) simulations on HECC systems in order to analyze unsteady aerodynamics and acoustics of proprotor-wing interaction, which is necessary to predict performance and noise generation/propagation for modern high-speed tiltrotors and advanced air mobility (AAM) aircraft with distributed electric propulsion.

Key Results

- The team established best practices for grid resolution, time step, turbulence model, and so on. Results were validated against experimental data from a standard wind tunnel test model for performance and a recent NASA wind tunnel test for aerodynamics and acoustics. The predicted thrust matched with the experimental data within 2% error for various operating and flow conditions.
- These validated CFD results provide confidence in the aerodynamic predictions and analyses in proprotor and wing interactions and are a stepping stone to move forward with acoustic predictions in the next year.

Role of HECC

- High-fidelity CFD simulations run on the Electra Skylake nodes enabled the team to predict complex propeller-wing flow fields at different operating conditions and determine physical sources of aerodynamic noise sources.

BENEFIT: This work supports NASA's Strategic Thrust 4: Safe, Quiet, and Affordable Vertical Lift Air Vehicles, by contributing to the ARMD strategic implementation plan mid-term (2025–2035) outcomes, which focus on "key technologies that will enable U.S. industry to expand the global vertical lift market while setting new standards in noise, safety, reliability, and performance."

"HECC provided invaluable resources to perform cutting-edge research in advancing technologies for VTOL vehicles. The accurate and detailed understanding of flow physics and the generation of valuable data achieved by this project could have not been achieved without support from HECC."
— Seongkyu Lee, University of California, Davis

Predicting Hypersonic Flows with Large-Eddy Simulations

Summary

- NASA Langley researchers are utilizing HECC resources to understand the extent that large-eddy simulations (LES) can be used for practical engineering applications, specifically as a potential replacement for experiments for wall-bounded turbulent reacting flows.

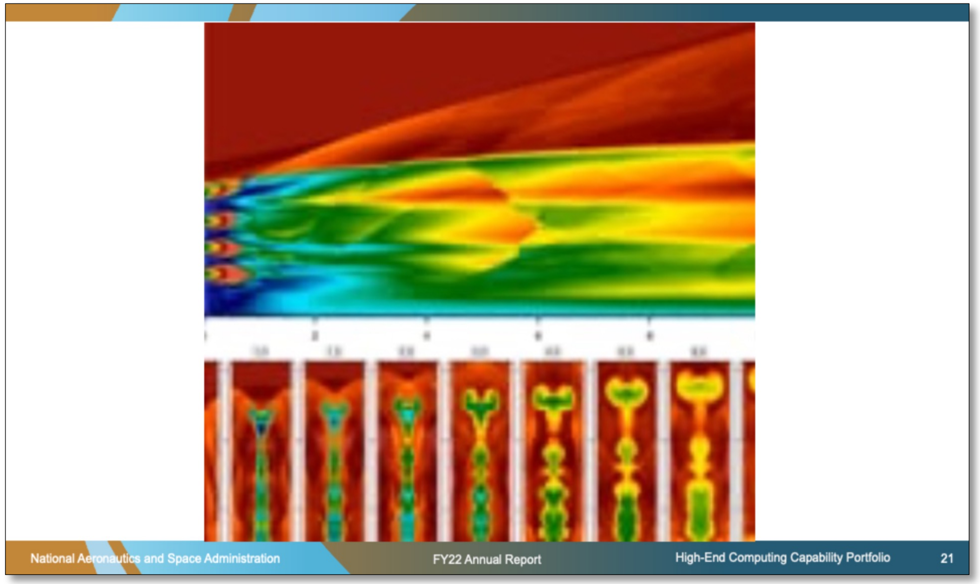
Key Results

- In FY22, the team performed several Reynolds-Averaged Navier-Stokes (RANS) simulations for a prototype scramjet combustor being developed by the Hypersonic Technology Project (HTP), then used LES and experiments to validate and verify the modeling parameters. Their optimization work demonstrated that the RANS/LES process can now be more routinely used by engineers for similar injector systems and for other flight conditions.

Role of HECC

- All the simulations performed for this work were primarily run on Pleiades and Electra Broadwell nodes. The team conducted 6,070 RANS simulations to build a surrogate model to be used in optimization, with each typically requiring 1,680 cores. Two LES simulations were also performed, utilizing 1,600 cores. Each simulation required about 1.5 terabytes of storage.
- During the course of the LES work, HECC staff supported the team with debugging of intermittent simulation failures that were traced back to the I/O, and provided the Langley team with a working solution to fix the issues.

BENEFIT: These computational fluid dynamics simulations contribute to advancing the state-of-the-art tools to understand and engineer ramjet and scramjet combustors for the next generation of high-speed propulsion systems for civil, military, and space applications.



"Without HECC resources, our computationally intensive optimization work, which produced the first generation combustor for an integrated propulsion system of a hypersonic prototype vehicle, would not have been possible." — Tomasz Drozda, NASA Langley

High-Fidelity Simulations for Multi-Rotor Urban Air Mobility

Summary

- Research scientists at NASA Ames, in support of the Revolutionary Vertical Lift Technology (RVLT) project, are providing high-fidelity data to study the agency's tiltwing and quiet-single main rotor (QSMR) air taxi concepts using the OVERFLOW/CAMRAD II loose coupling methodology. These datasets can be used to improve the empirical models used by current urban air mobility (UAM) vehicle design tools.

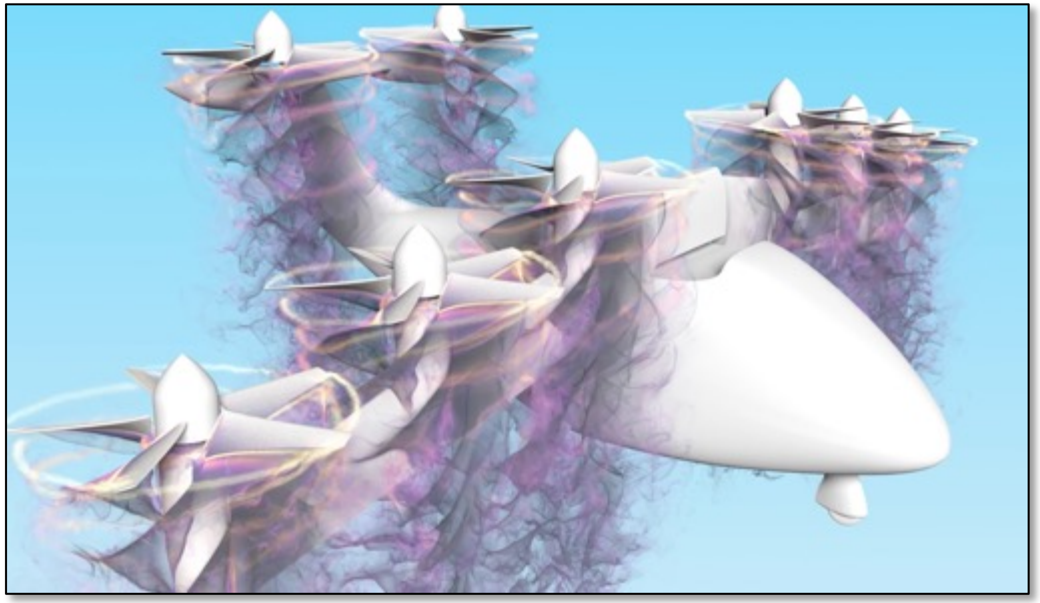
Key Results

- The team investigated the acoustics of three different rotor designs for the QSMR helicopter and discovered that drooping the tip and lowering the tip speed substantially reduced tonal noise while maintaining hover performance. However, this design change significantly decreased cruise efficiency, demonstrating the trade-off between noise reduction and overall performance.
- Flow visualizations were helpful in understanding the complex aerodynamic interactions between the tiltwing vehicle's rotors, wake, and airframe. Such interactions reduced the performance of the wing inboard propellers. The results obtained through computational fluid dynamics are essential given the limited availability of experimental data.

Role of HECC

- HECC provided the supercomputing resources and services in support of this work. Simulations used 1,000-3,000 processors and took 10–20 days.

BENEFIT: High-fidelity CFD simulations of RVLT concept vehicles contribute to NASA's mission and research in Urban Air Mobility by analyzing and studying key vehicle components and configurations—ultimately helping in the design of safe, efficient, and quiet UAM vehicles.



"HECC project resources are essential for this work, and its visualization team generates high-resolution images and videos that aid in viewing and analyzing complex flows."
— Patricia Ventura Diaz, NASA Ames

Materials Modeling for Environmental Barrier Coatings

Summary

- Researchers at NASA Glenn performed simulations to calculate properties of environmental barrier coating (EBC) candidate materials, in order to improve understanding and accelerate development of coating systems for gas turbine engines. In one of several studies, the Glenn team developed and validated the only known machine learning-derived interatomic potentials (IAPs) for two state-of-the-art EBC materials, yttrium disilicate (YDS) and ytterbium disilicate.

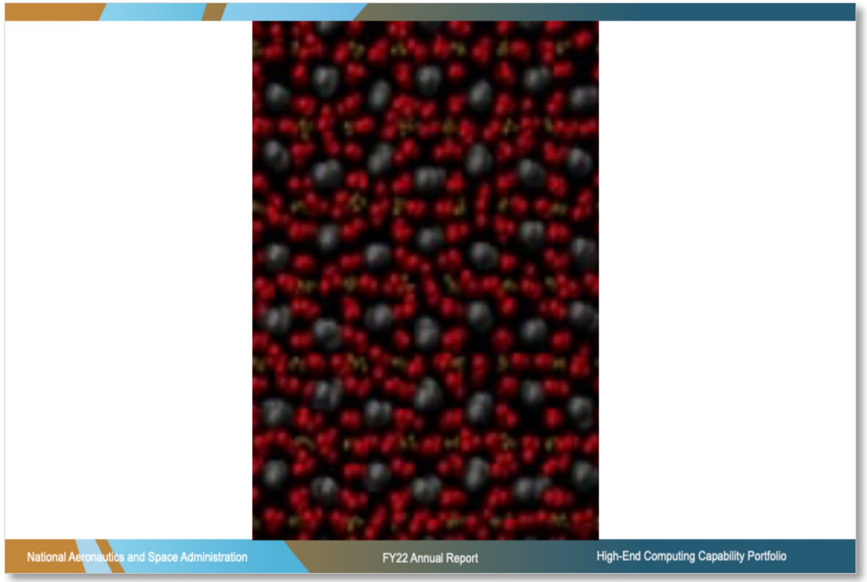
Key Results

- The IAPs enabled simulations of material lattice properties and thermodynamic properties at near-density functional theory (DFT) accuracy with orders-of-magnitude speedup over a state-of-the-art DFT code.
- Simulations using the YDS IAP correctly predicted both the three unique crystal phases of YDS and the anisotropy of thermal expansion seen experimentally in X-ray diffraction studies.
- Results from another study showed that EBCs electronic structure changed as a function of dopant concentration, which can help to guide coating design.

Role of HECC

- HECC supercomputers enabled thousands of individual density functional simulations to correlate electronic structure to material properties and to produce training and validation data for IAP development.

BENEFIT: These simulations will enable researchers to calculate material properties that were previously intractable, providing more information for environmental EBC system designers. Optimized EBCs will, in turn, enable increased fuel efficiency in aircraft gas turbine engines—directly benefitting NASA's goals to increase engine efficiency and decrease environmental impacts.



"The high-throughput capabilities of HECC resources significantly decreased the time required to perform the simulations in this work."

— Cameron Bodenschatz, NASA Glenn

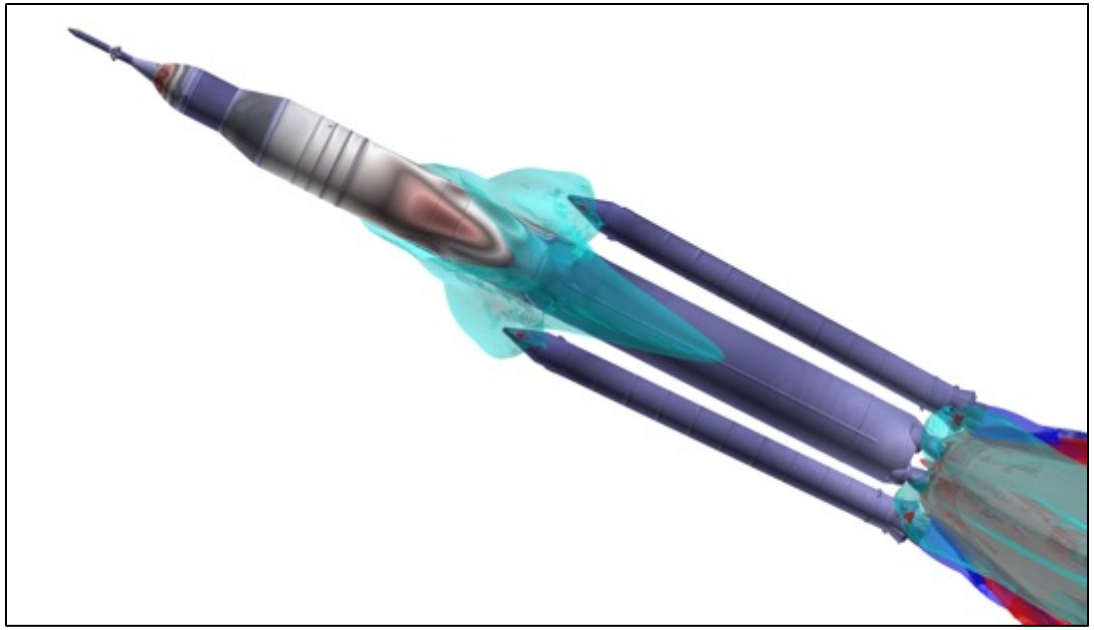
National Aeronautics and
Space Administration

HECC Annual Report FY22

Human Exploration and Operations Mission Directorate

HECC FY22: Space Technology, Exploration, & Operations

- NASA's vision for the Artemis Program, as well as human exploration of Mars and key innovations for safe, sustainable space exploration rely on comprehensive modeling and simulation made possible by HECC supercomputing resources and array of technical expertise.
- In FY22, the investment in HECC systems and services supported 94 STMD, SOMD, ESDMD, and NESC projects, providing engineers and scientists with over 30 million SBUs* to meet their program objectives.
- Ten representative projects are highlighted, ranging from supporting the successful Artemis I flight test and providing continuing support to the Artemis Program, to investigating new metal alloys for 3D printing manufacturing and new composite materials for launch vehicles, to developing software tools for entry systems modeling and plume-surface interactions. These projects contributed to several program-level reviews and milestones and produced more than 70 publications, presentations, and reports during this period.
- Looking ahead, HECC resources and services will continue to play a key role in Artemis Program missions that will return humans to the Moon—and help pave the way for human exploration of Mars.



**1 SBU equals 1 hour of a Pleiades Broadwell 28-core node.*

HECC FY 2022: Space Exploration, Technology, and Operations

- **Total Usage: 30,884,769 SBUs**
  - **Number of Projects:** 94
  - **Average CPU Range:** 8,193 – 16,384 CPUs
  - **Average Expansion Factor:** 2.15
  - **Share:** 34,529,360 SBUs
  - **Usage as Percent of Share:** 89%

- **By Mission Directorate/Program**

Exploration Systems Development (ESDMD) 16,954,017

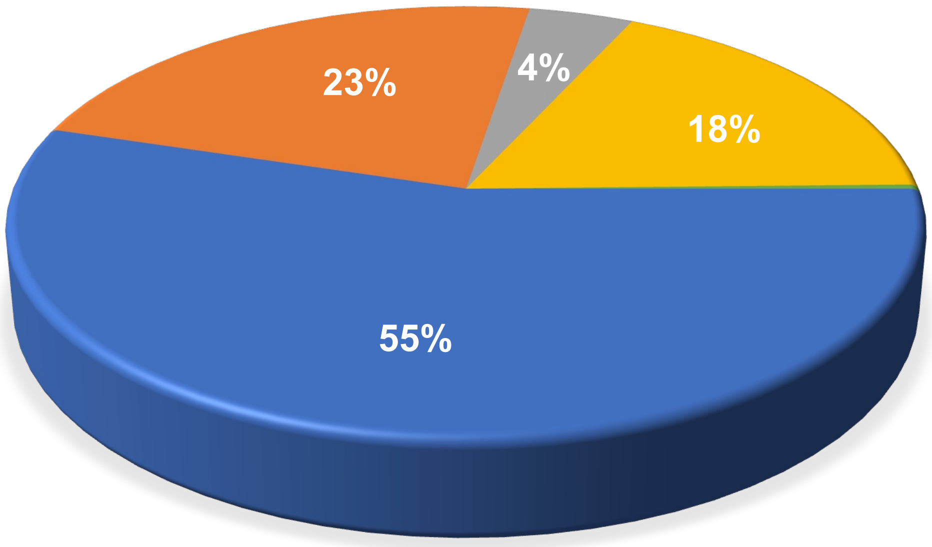
Space Technology (STMD) 7,089,024

NASA Engineering & Safety Center (NESC): 5,509,672

Space Operations (SOMD): 1,332,056

Human Exploration and Operations (HEOMD): 98,092

HEOMD FY22 Usage



**1 SBU equals 1 hour of a Pleiades Broadwell 28-core node.*

Development of Metal Alloys for 3D Printing Applications

Summary

- As part of the Refractory Alloy Additive Manufacturing Build Optimization (RAAMBO) project, researchers at NASA Ames are using quantum mechanics simulations run on HECC systems to understand the properties of metal alloy compositions for use in additive manufacturing of high-temperature parts like rocket nozzles.

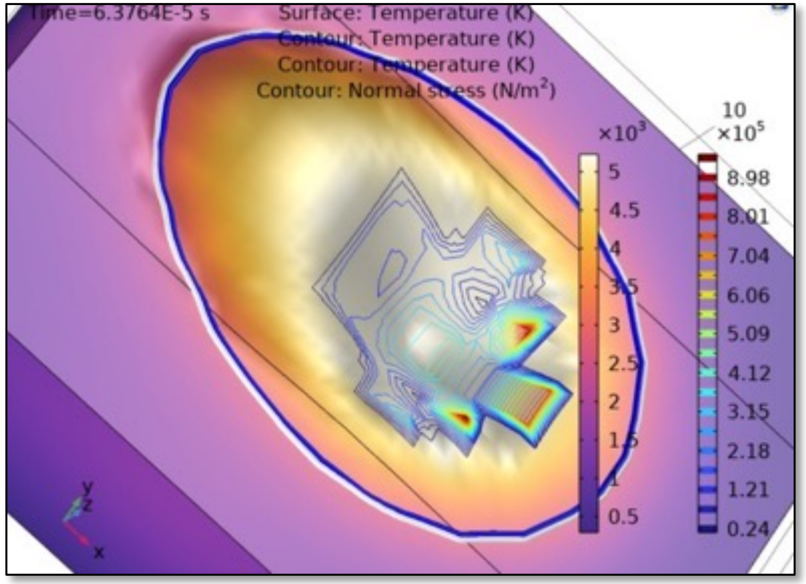
Key Results

- Since the alloys will be used by the agency in 3D printing manufacturing processes, it is important that the materials retain their properties at high temperatures and can produce parts without defects. The results of the simulation work done by the team at Ames was used to inform higher-scale process modeling, helped to develop the experimental printing process, and is being used to guide the printing of rocket nozzle designs for tests.

Role of HECC

- Characterizing the performance of an alloy for additive manufacturing requires computationally intense quantum mechanical simulations of electronic and atomic structures. With simulations requiring tens of thousands of node hours on the Pleaides supercomputer, the team ran molecular dynamics, density functional theory, and Monte Carlo simulations to predict material properties that were not available from laboratory data.

BENEFIT: This work is part of an effort to develop alloys that can be used in the additive manufacturing of high-temperature parts such as rocket nozzles, which can reduce manufacturing costs and allow for the rapid prototyping of efficient designs that are not possible with traditional fabrication techniques.



"HECC resources allow the performance of computationally intense, quantum mechanical simulations over a wide range of compositions and conditions, accelerating the identification of candidate compositions."
— ***Justin Haskins, NASA Ames***

Modeling Nanostructured Composites for Launch Vehicles

Summary

- A team at NASA Langley is using HECC resources to perform atomistic simulations for the development of polymer matrix/carbon nanotube yarn composites. High-performance materials for next-generation aerospace vehicles have traditionally been developed using an iterative, empirical process, but this effort seeks to use state-of-the-art quantum mechanical and classical molecular dynamics techniques to accelerate the development of nanostructured composite materials for launch vehicle applications.

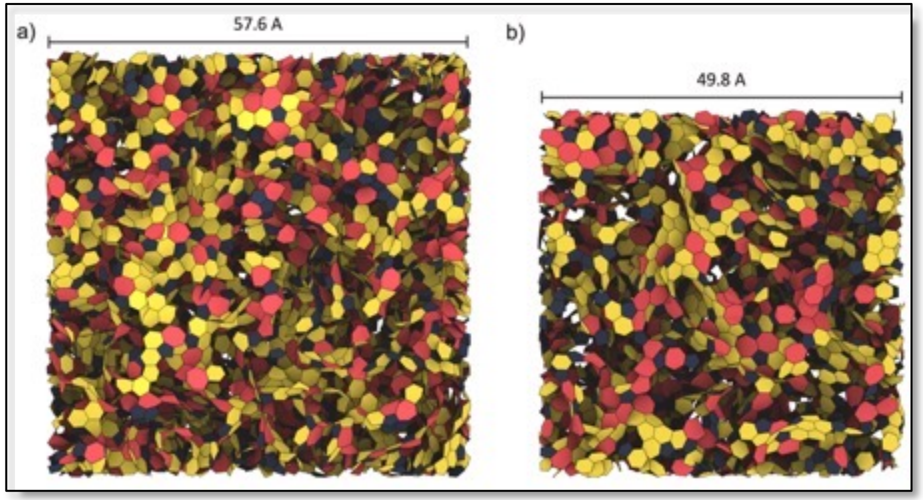
Key Results

- From initial polymerization to mechanical fracture under load, the team used computational methods to simulate several relevant phases of the functional life of polymers and composite materials. Molecular dynamics simulations allowed them to model and predict material behavior when exposed to specified temperatures, pressures, and applied strains.

Role of HECC

- The team ran their simulations on the Pleiades supercomputer, which enabled them to collaborate with experimental synthetic and characterization work. This computationally intensive work has helped to accelerate the development of new chemistries by predicting which are most likely to meet project requirements, and can only be completed with high-performance computing resources.

BENEFIT: NASA relies on the emergence of new materials that enable the realization of vehicle designs that sometimes cannot be constructed using existing materials in a safe or affordable manner. This work seeks to fill the gap by developing tools that allow rapid exploration and simulated testing of new materials for future aerospace missions.



"HECC resources enabled the numerous and lengthy simulations required to explore the parameter space of materials with the potential to meet the structural and thermal requirements for use in future exploration vehicle applications."

— Kristopher Wise, NASA Langley

Simulations Provide Crucial Support for Artemis Program

Summary

- Computational fluid dynamics (CFD) simulations run by aerospace engineers at NASA Ames play a crucial role in designing and certifying the different families of Space Launch System (SLS) configurations. The simulations, run on HECC resources, focus on the first few minutes of the ascent, when aerodynamic forces and pressures play a major role in the vehicle's ability to maintain controlled flight without damaging or destroying the vehicle or any of its components.

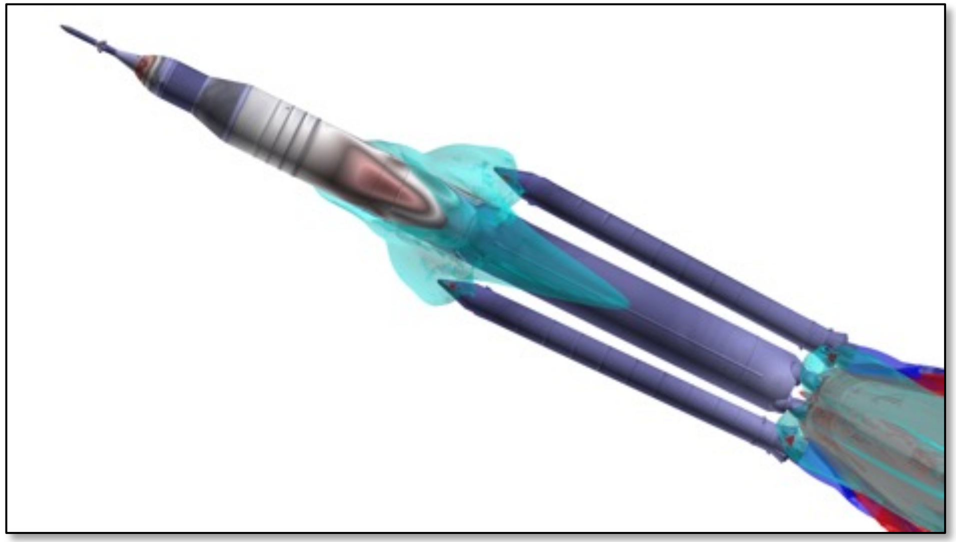
Key Results

- The Ames team ran tens of thousands simulations of the Artemis IV Block 1B vehicle during booster separation; performed detailed geometry trade studies; developed a fine-resolution CFD model of the Artemis I vehicle; and ran debris transport simulations in support of Artemis I launch preparations.
- Their debris transport analysis provided critical data on the risk of potential debris, including risks from hurricane damage, along with rapid day-of-launch debris assessments. The fine-resolution CFD model of Artemis I will be used in the post-flight analysis and comparison to flight data.

Role of HECC

- The steady and time-accurate Reynolds-Averaged Navier-Stokes CFD simulations, which use high-fidelity computer models together with wind-tunnel data, would not be possible without HECC resources.

BENEFIT: The simulation data are critical to the design, construction, and flight of the Space Launch System family of vehicles. In FY22, this work directly supported the successful Artemis I test flight objectives, as well providing aerodynamic data for the Artemis IV and subsequent flights to help ensure these missions will be flown safely.



"HECC resources enable our team to produce critical aerodynamic data using high-fidelity simulations, including data that could not be obtained by any other method. In addition, without them, the SLS Program would have to rely on far more expensive and time-consuming wind tunnel testing." — ***Stuart Rogers, NASA Ames***

Developing Software Tools for Entry Systems Modeling

Summary

- Researchers supporting NASA's Entry Systems Modeling project develop modeling and simulation tools that will enable new entry system capabilities across the solar system, improve performance, and reduce mission risk. Project tasks are spread across four core technical areas: thermal protection system (TPS) material modeling; shock layer kinetics and radiation; aerosciences; and guidance, navigation, and control.

Key Results

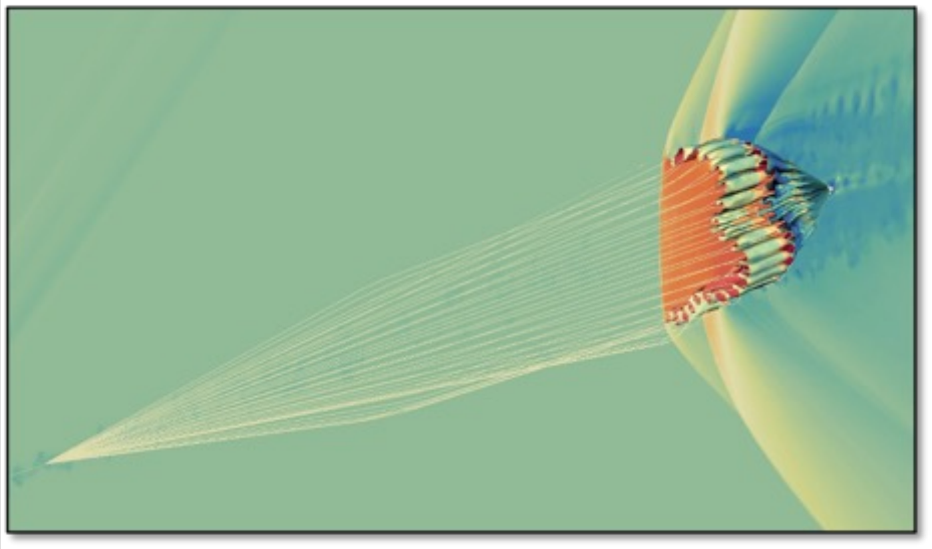
- The team built and verified Icarus software, resulting in its use in the Dragonfly and Mars Sample Return Earth Entry System flight projects for multi-dimensional modeling of TPS performance. They also developed Massively Parallel Electron Correlation—the only tool available that can calculate the complex electronic structure of diatomic and triatomic molecular interactions at energies relevant to entry.

- The team simulated the ASPIRE parachute flight tests for supersonic deployment at Mars; results showed good agreement with flight data.

Role of HECC

- Extensive simulation development, validation, and production runs using grids ranging from 10- to 100-million cells were carried out on Pleiades, using around 1,000 cores, with a typical wall-clock time of approximately four to eight days per run.

BENEFIT: NASA's investment in computational tools will guide next-generation EDL design with quantified uncertainty for performance and risk management. Advanced simulation technology is a key path toward enabling missions to achieve their requirements within acceptable technical risk and cost constraints.



"All of the tools used by the Entry Systems Modeling project are built on high-performance, distributed computing paradigms. Simply put, they would not work without access to HECC resources."
— Michael Barnhardt, NASA Ames

Multi-Scale Modeling of Plume-Surface Interactions

Summary

- The success of future lunar and planetary exploration missions requires predictive simulation tools that capture the complex multiphase dynamics associated with rocket exhaust impingement during lunar and planetary touchdown. Researchers at the University of Michigan (U-M) are developing advanced physics-based models and numerical algorithms to enable predictive simulations of plume-surface interactions in landing conditions.

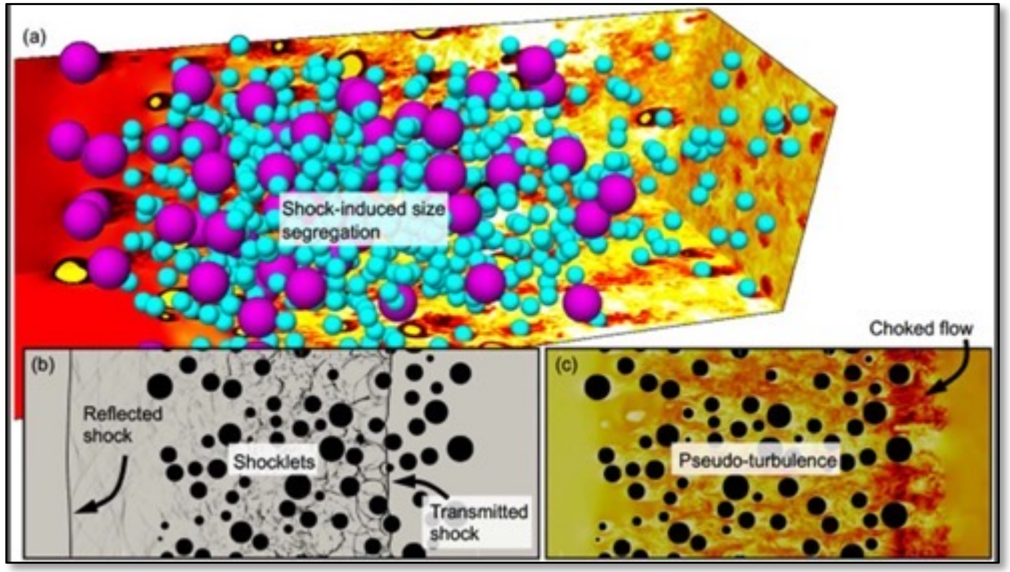
Key Results

- In FY22, the U-M team developed the first drag model relevant for compressible flows in particle suspensions; that is, the drag force in flows containing multiple interacting particles at finite Mach number.
- The budget of turbulent kinetic energy during shock-particle interactions was also quantified. This revealed how drag induced by particles is the primary production mechanism of turbulence in dense suspensions, which is mainly balanced by viscous dissipation. These results are being used to develop a novel two-equation transport equation for particle-induced turbulence.

Role of HECC

- Simulations of compressible flows through assemblies of solid particles, and particle-resolved simulations of a planar shock interacting with a curtain of particles, were run on the Pleiades supercomputer. In addition, Eulerian-Lagrangian simulations of particles in under-expanded jets were performed and validated against experiments at Johns Hopkins University.

BENEFIT: This work supports NASA's development of Eulerian-based two-fluid models for simulating plume-surface interactions that occur when spacecraft land on the Moon and on planets**.** The simulations are designed to shed light on the flow physics taking place at the microscale and inform new models to improve the validation range that two-fluid models are used for.



"HECC resources allow us to develop, test, and perform high-fidelity simulations of complex flows with unprecedented detail."
— Jesse Capecelatro, The University of Michigan

Nucleate Boiling Heat Transfer Mechanisms in Microgravity

Summary

- Researchers at the University of Maryland, College Park ran high-fidelity direct numerical simulations (DNS) on Pleiades to improve the modeling of fundamental physical mechanisms associated with nucleate boiling for thermal management in different gravity environments, ranging from orbiting vehicles to future missions to Mars and beyond.
- The team simulated the experimental conditions of the Microheater Array Boiling Experiment and Nucleate Pool Boiling eXperiment to obtain detailed characterization of the highly complex evolution of bubble dynamics and the associated heat transfer mechanisms.

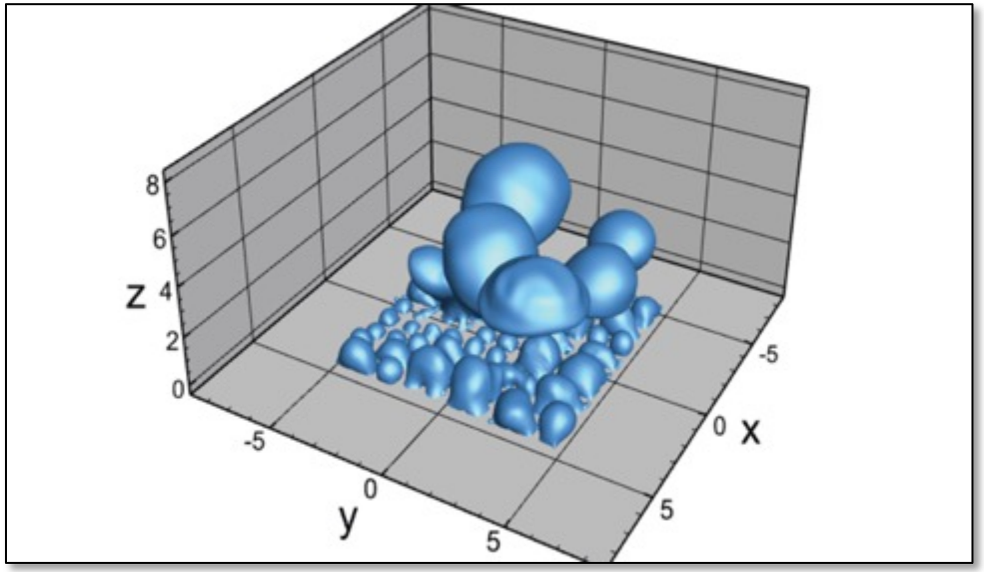
Key Results

- Multiple modes in the bubble size distribution for higher subcooling levels were observed compared to single-mode narrow concentration of smaller bubbles for low subcooling levels at steady state. To date, the simulations confirm experimental findings that biphilic surfaces (with hydrophobic patterns on hydrophilic structures) can lead to relatively large improvements in heat transfer compared to a purely hydrophilic surface.

Role of HECC

- Each simulation provided high-resolution definition and visualization of prominent flow features over a broad range of spatio-temporal scales, using 1,000 Pleiades Broadwell cores for over 200,000 processor hours.

BENEFIT: This project will produce the essential data that connects heat flux to the dynamics of nucleate boiling under a range of gravity conditions, providing a unique opportunity to assess fundamental thermal mechanisms and enabling key improvements in the design of thermal protection systems for spacecraft used in NASA missions ranging from low-Earth orbit to the Moon and Mars.



"HECC's Pleiades supercomputer, along with our leading edge computational methods, enables us to carryout high fidelity simulations with unprecedented precision."
— ***Amir Riaz, University of Maryland, College Park***

Machine Learning to Predict Solar Proton Event Hazards

Summary

- Heliophysicists at Georgia State University, New Jersey Institute of Technology, and NASA Ames use HECC resources to enhance the capability to predict solar energetic particles (SEP) by implementing automatic data characterization and machine-learning tools. They aim to develop the capability to create robust "all-clear" forecasts of solar proton events (SPEs) with low false-alarm rates, targeted at different temporal scales, energy and particle flux thresholds, and adapted to operational availability of data sources and gaps.

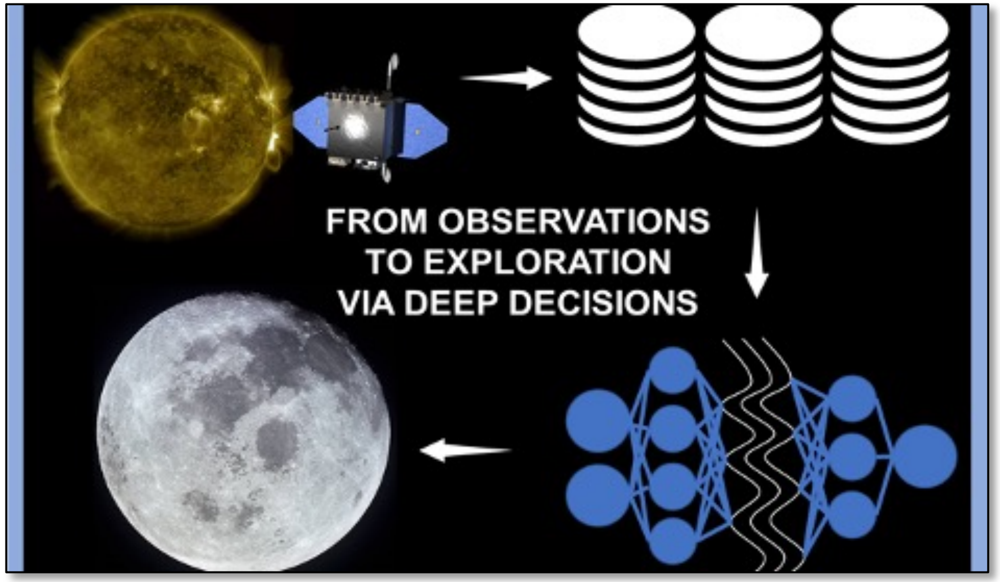
Key Results

- In FY22, the researchers made significant process toward developing an online database that integrates solar/heliospheric data, metadata, and descriptors related to SPEs.
- The team investigated cross-cycle transferability of the forecasts of SEPs based on statistical properties of the GOES Soft X-Ray and proton fluxes; created a homogeneous dataset of McIntosh and magnetic classes of solar active regions for 1981–2020; and developed flare-driven SPE prediction based on random forest and neural network-based random hivemind (RH) approaches.

Role of HECC

- HECC provides the ability to customize machine learning environments for efficient data analysis of massive multi-dimensional datasets. Project achievements are based on the Interactive Multi-Instrument Database of Solar Flares and the Radiation Data Portal, hosted in HECC's Data Portal.

BENEFIT: This project contributes to NASA's effort to develop a robust methodology for predicting solar energetic particle hazards, directly addressing research Goals 1 and 4 of the Decadal Survey for Solar and Space Physics. Predicting hazardous radiation that affects astronauts is a crucial component for the success of NASA's Artemis missions.



"HECC's computational resources and machine learning tools enabled this work." ***— Alexander Kosovichev, New Jersey Institute of Technology***

Predicting Crater Ejecta from Plume-Surface Interaction

Summary

- To fill the large gaps in our understanding of the physics involved during supersonic plume interaction with granular soil on planetary surfaces during controlled landing, scientists at NASA JPL developed a new model describing soil crater formation and the resulting ejecta formed during this process, with direct relevance to the Artemis Program. Ejecta has the potential to damage the lander and harm astronauts.

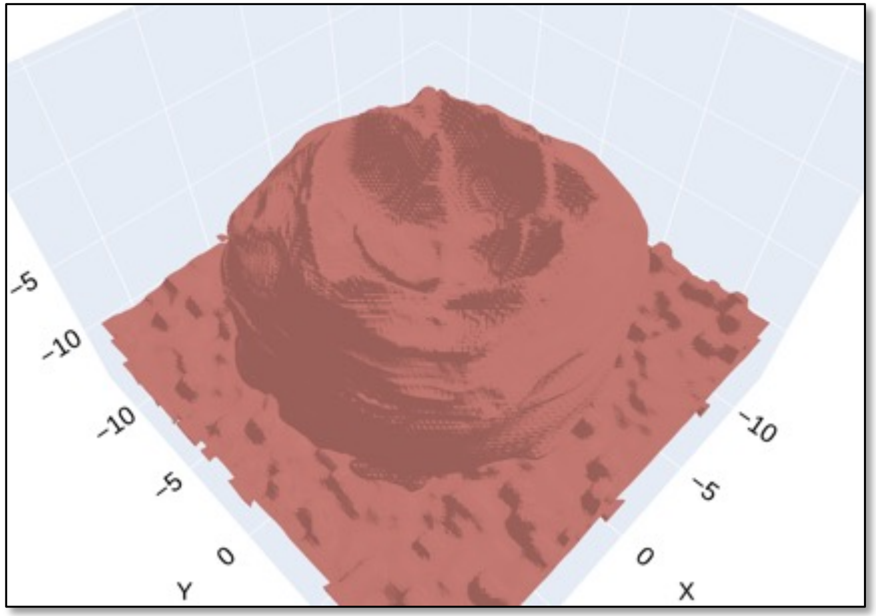
Key Results

- The JPL team validated their new model of the governing equations that is hyperbolic, and performed production runs on HECC systems to explain the importance of the parameters that control various aspects of the physics. These achievements are substantial—the interaction of the plume with the soil creates pressure waves, which cannot physically propagate through the soil unless the set of governing equations is hyperbolic.
- The crater ejecta predicted by the model are a quantitative measure of what will happen in reality should the simulations be scaled from the present fundamental study to a practical situation. This is the first set of hyperbolic equations for three-dimensional unsteady granular flows.

Role of HECC

- The JPL team ran production simulations on HECC systems, which have been essential to obtaining their results.

BENEFIT: This model provides a quantitative measure of what will happen in reality should the simulations be scaled from the present fundamental study to a practical situation. This would impact lunar missions, such as Artemis; and it is directly applicable to Mars and other space bodies with atmospheres having different compositions and pressure, such as, Titan.



"We simply would not have been able to do this work without HECC resources."

— Josette Bellan, NASA JPL

Engineering Risk Assessment for Space Exploration

Summary

- This year, the Engineering Risk Assessment (ERA) team at NASA Ames applied its physics-based modeling and simulation with probabilistic risk assessment techniques to gain insight into phenomena that could contribute to large-scale explosions of the Space Launch System (SLS), with a focus on flame acceleration following ignition of a flammable mass of gas accumulated within a confined volume.

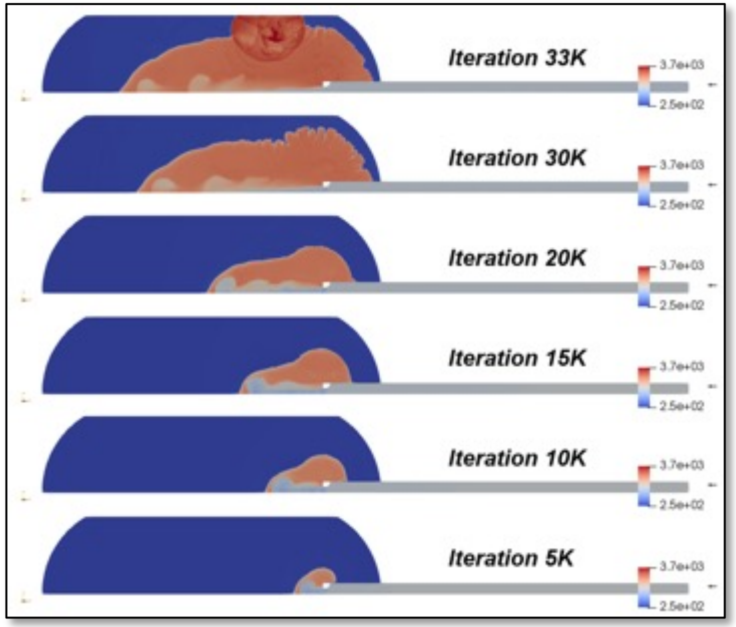
Key Results

- The team successfully ran simulations of hot, burned gas jetting into unburned hydrogen/oxygen/nitrogen mixtures to assess the potential for flame acceleration to detonation. Sensitivities performed included varying chamber temperature, pressure, and density, as well as levels of nitrogen.
- They also performed simulations of high-speed fragment impact on a thin-walled spherical vessel under internal pressure. Results are interpreted in terms of impact velocity decrement, whether the target hole remains stable, and, if not, the speed of the subsequent crack growth.

Role of HECC

- The insights provided by these fundamental physics simulations were enabled by HECC supercomputing resources, and provide guidance in the specification of inputs for subsequent modeling.

BENEFIT: The insights provided by these fundamental physics simulations provide guidance for the specification of inputs for subsequent modeling within the abortability table generation process, and ultimately help characterize explosion environments that pose threats to crews.



"The physics underlying the unique classes of behavior associated with SLS system failure modes is complex and requires high-fidelity simulation such as can only be provided by computing systems such as those provided by HECC." — ***Ashley Coates, NASA Ames***

Simulating Fluid Dynamics for Spacecraft Engines

Summary

- Researchers at NASA Marshall support a variety of cryogenic fluid management (CFM) and turbomachinery computational fluid dynamics (CFD) applications for aerospace vehicles across the agency, including the Human Lander System (HLS) Program. Utilizing HECC resources, the team developed CFD and volume of fluid models to represent vapor and liquid phases to validate cryogenic propellant tank self-pressurization; as well as time-accurate combusting CFD analyses of rocket engine injectors to assess the probability of non-uniform or incomplete combustion that might cause engine test failures.

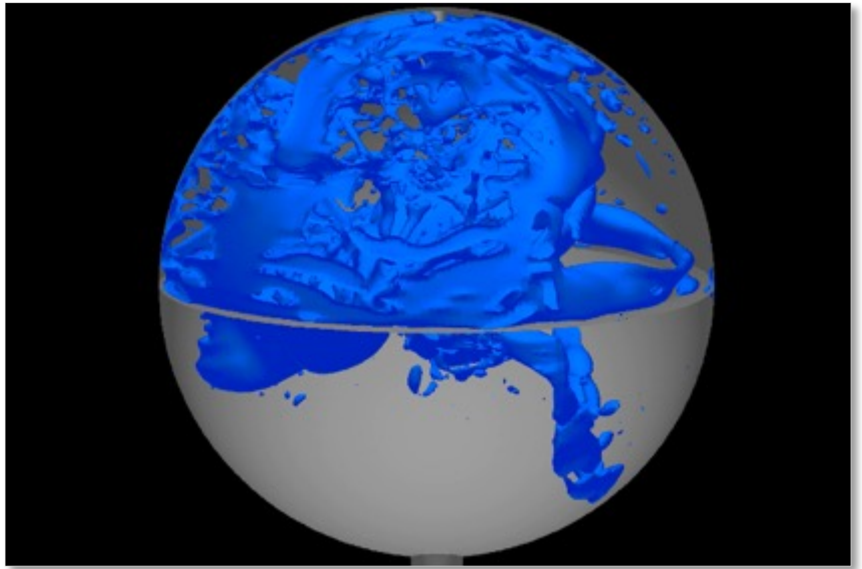
Key Results

- The results from the HLS reacting flow simulations provided heat flux predications to the combustion chamber wall for operational and design considerations, and the CFD output will be used as input for separate, pre-test combustion stability calculations.
- Successful validations were performed for CFM applications that will inform simulations of future agency and partner spacecraft operations. Propellant-mixing simulations demonstrated sufficient performance to enhance thermal vent system operation for a Commercial Lunar Payload Services partner.

Role of HECC

- These parametric and large-scale studies required concurrent simulations over weeks, which would not have been possible without HECC resources.

BENEFIT: This work enhances NASA's understanding of methods used to control propellant distribution during a variety of in-space vehicle maneuvers, and improves reacting flow modeling and combustion stability prediction tools. This enables more informed design solutions for spacecraft and evaluation of existing designs.



"HECC staff worked with analysts to optimize model efficiency through appropriate resource utilization. The computational resources made available to the project were crucial to achieving schedule milestones and enabled the subject simulations." — ***Jacob Brodnick, NASA Marshall***

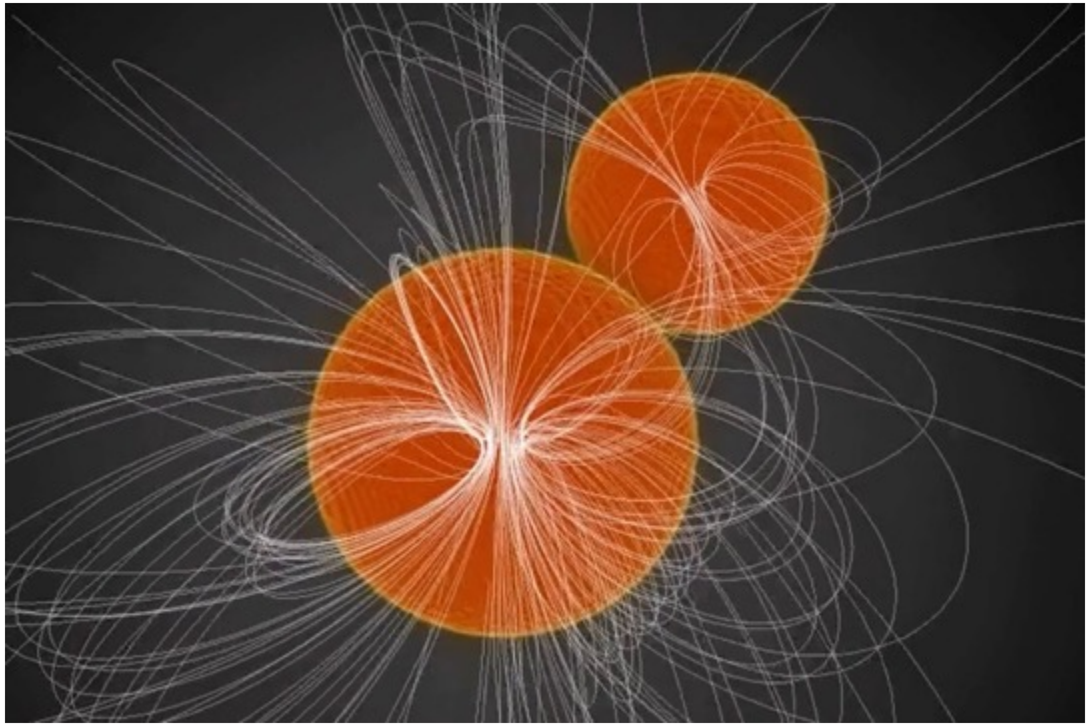
National Aeronautics and
Space Administration

HECC Annual Report FY22

Science Mission Directorate

HECC FY22: Science Mission Directorate

- NASA's leadership role in seeking knowledge and deep understanding of our planet, solar system, and the universe relies on HECC supercomputing resources and technical expertise to support all areas of the agency's science mission.
- In FY22, the investment in HECC systems and services supported 580 SMD projects, providing scientists and engineers with more than 70 million SBUs* to meet program objectives.
- Twenty representative projects are highlighted, including simulations for: improving our knowledge of the global carbon cycle and quantify changes in atmospheric CO_2; investigating the orbits, sizes, and impact rates of near-Earth objects; improving space weather modeling; exploring black hole physics; and maintaining the science processing operations pipeline for the NASA Explorer Program's Transiting Exoplanet Survey Satellite (TESS) Mission.
- These 20 projects produced more than 100 publications and presentations that collectively earned hundreds of citations.
- HECC resources and services will continue to play a key role in interpreting data from observatories including TESS, the James Webb Space Telescope, and the Surface Water and Ocean Topography (SWOT) mission, launched in January 2023; advancing understanding of the sea-level rise and other effects of climate change; and enabling scientific discovery on Earth and beyond.



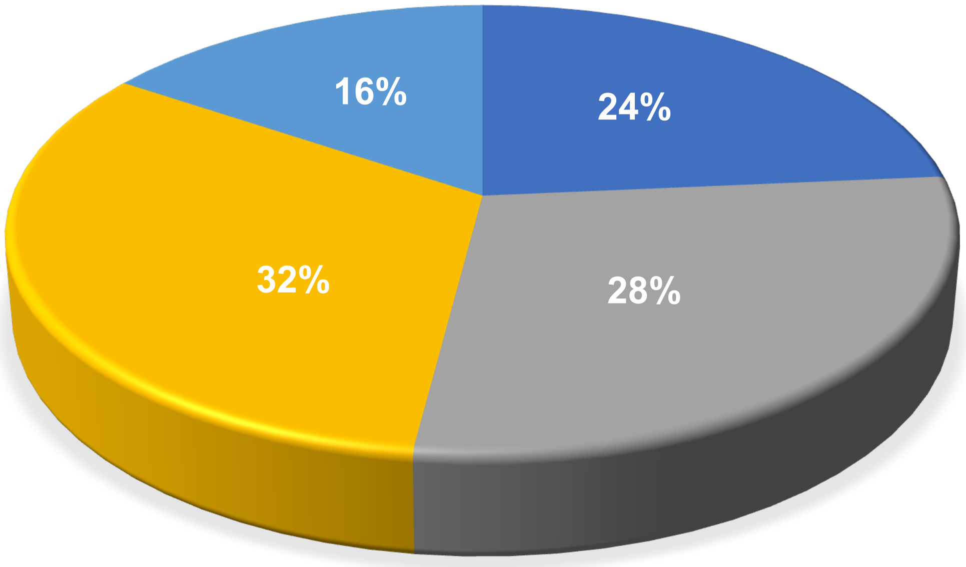
**1 SBU equals 1 hour of a Pleiades Broadwell 28-core node.*

HECC FY 2022: Science Mission Directorate

- **Total Usage:** 70,478,607 SBUs
  - **Total Number of Projects:** 580
  - **Average CPU Range:** 16,385 – 32,768 CPUs
  - **Average Expansion Factor:** 2.07
  - **Agency Reserve:** 8,405,394 SBUs
  - **Share:** 56,820,467 SBUs
  - **Usage as Percentage of Share:** 124%
  - **Usage as Percent of Share + Agency Reserve:** 93%
- **By Program**

  - **Heliophysics:** 22,834,566
  - **Earth Science:** 20,041,297
  - **Astrophysics:** 16,621,369
  - **Planetary Science:** 10,981,374

SMD FY22 Usage



**1 SBU equals 1 hour of a Pleiades Broadwell 28-core node.*

New Findings on Magneto-Rotational Instability in the Sun

Summary

- To improve understanding of the origin of the solar magnetic field, researchers at Northwestern University are running a series of numerical calculations to investigate whether the magnetic field is generated in the Sun's near-surface shear layer. The research team develops numerical techniques for running simulations in spherical geometry—including radiative transfer—and for data assimilation to make better predictions of solar magnetism.

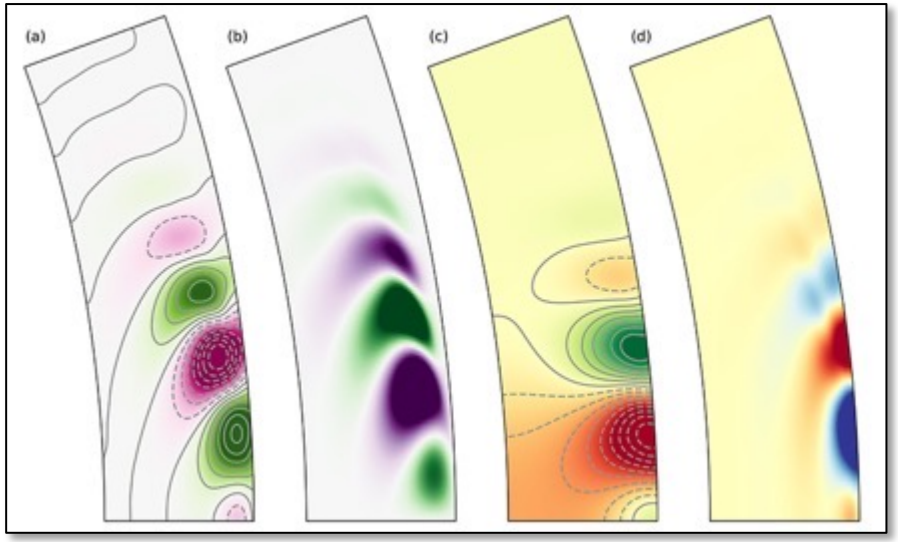
Key Results

- The team has found the first large-scale magneto-rotational instability in the solar near-surface shear layer, and is studying the effects of this instability to determine how or if it is connected to solar magnetism.
- They implemented a two-dimensional eigenvalue solver within the open-source Dedalus pseudo-spectral framework to efficiently calculate linear instability modes of the Sun. This method is significantly faster than previous methods to find unstable modes.

Role of HECC

- HECC resources made it easy to develop, test, optimize, and run production-scale numerical calculations; and enable work with Dedalus for large-scale computations to efficiently calculate linear instability modes. HECC experts optimized parts of the Dedalus code to run these simulations.

BENEFIT: The solar magnetic field drives space weather, which can have significant consequences on Earth—affecting radio waves, GPS satellites, computers aboard spacecraft, and more. These numerical techniques and the new theory of instability in the near-surface shear layer are key to making accurate predictions of solar magnetism.



"Our work is only possible with HECC resources. It has underpinned all the results of this project, and many other projects I have participated in. I find it significantly easier to use HECC resources than other national supercomputers, and it allowed us to produce better results more quickly."
— Daniel Lecoanet, Northwestern University

Understanding Carbon-Climate Relationships

Summary

- As part of NASA's goals to improve understanding of the global carbon cycle and quantify changes in atmospheric CO_2, researchers at NASA JPL are utilizing computational resources provided by HECC to understand the implications for long-term changes in the terrestrial biosphere carbon cycle with changes in climate.

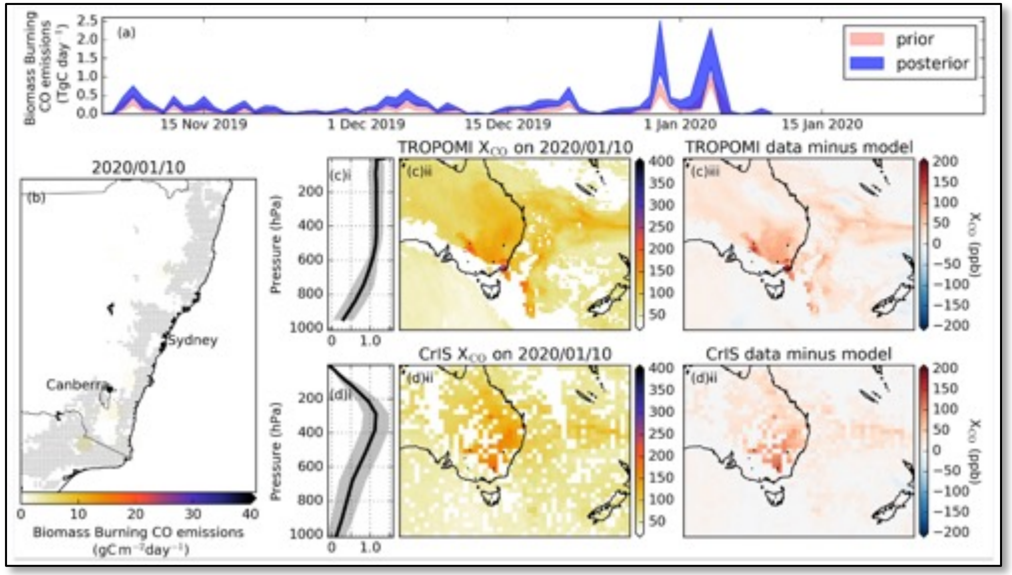
Key Results

- The team carried out global, top-down CO_2 flux inversions during 2015–2021, using samples taken from aircraft and observations from an orbiting carbon observatory. They tested regional inversions over Africa at high resolution to estimate carbon changes due to biomass burning and seasonal behavior.
- They also performed regional inversions over Australia using space-based measurements to quantify the carbon cycle anomalies resulting from drought and fire during the 2019–2020 growing season. Their results showed that these events reduced carbon uptake and produced more carbon than Australia's annual fossil fuel emissions.

Role of HECC

- The computational resources provided by HECC, in addition to the storage and software support, allowed the JPL team to optimize their flux inversion system to reduce wall-clock time in order to run their simulations and perform experiments to quantify the impact of satellite flux on inversion results.

BENEFIT: Using observations from multiple satellites and and a data assimilation terrestrial biogeochemical model, this work advances our understanding of the global carbon cycle from an Earth system perspective.



"The 24-hour support provided by HECC enabled quick fix of any problem our group had, which has improved the efficiency of our work. The large storage provided enabled the group to run multiple experiments to test different sensitivities, and the software provided made data analysis convenient to carry out."

— Junjie Liu, NASA JPL

An Integrated Approach to Barystatic Sea-Level Projections

Summary

- Scientists at NASA JPL improved the agency's capability to model and make projections to better understand various phenomena that affect relative sea ice level—including ocean circulation around the Antarctic ice sheet, interactions between solid-Earth and the cryosphere, interactions between ice sheets and the atmosphere, as well as coastal area positions and migration. They relied on uncertainty quantification (UQ) and the Ice-Sheet and Sea-Level System Model (ISSM).

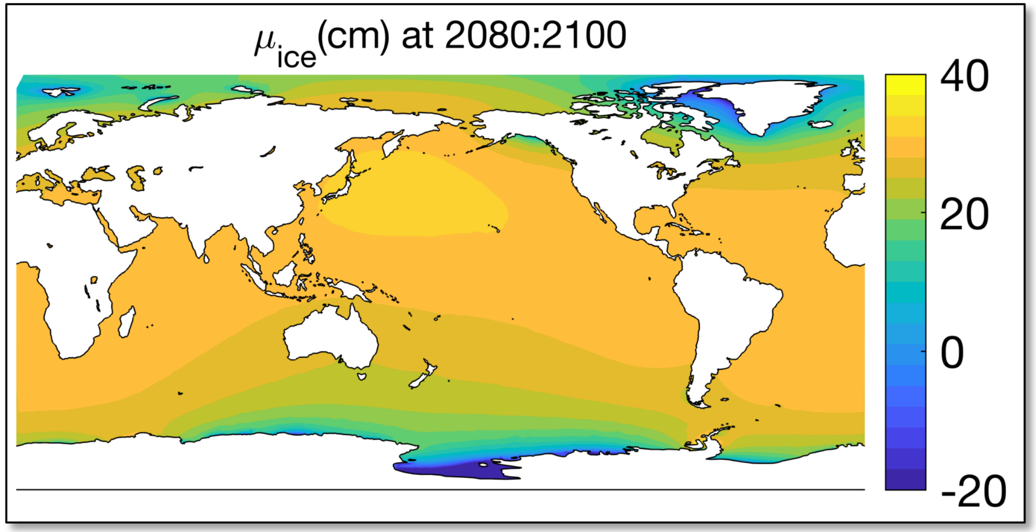
Key Results

- The JPL team achieved new projections with ISSM that will be relied on by the NASA Sea-Level Change Science Team to improve on projections used in the United Nations Intergovernmental Panel on Climate Change Sixth Assessment Report framework. They also attained unprecedented sensitivity analyses of the impact of the presence of rifts on ice shelf melt rates and under-cavity oceanic circulation.

Role of HECC

- Computations were run on the Pleiades supercomputer to make projections of sea level rise in centimeters by the year 2100 using ISSM and a UQ approach. This involved significant runs to sample the projection space (several thousand samples for runs that take 2–3 minutes per sample on 250 processors each); and ocean circulation on Larsen C ice shelf for 20 years, full representation of rifts in the ice shelves, using the MIT general circulation model.

BENEFIT: This work will improve NASA's ability to project sea-level rise using all of the agency's remote sensing and modeling capabilities. The impact will be interagency, with potential interest from other teams at the National Oceanic and Atmospheric Administration.



"HECC resources allowed for an unprecedented 10-km resolution in our gravity, rotation, deformation representation of sea-level projections at the coastline, while still being able to run projections for 100 years, using a sample set size of 2,000 samples, which is also is unprecedented."
— Eric Larour, NASA JPL

Accelerating Earth Science Research via the NEX Infrastructure

Summary

- Using HECC's state-of-the art supercomputing resources, NASA-funded Earth scientists explore and analyze terabyte-to-petabyte-scale datasets and advanced modeling at regional, continental, and/or global scales. NASA Earth Exchange (NEX) scientists supported data management, code development, and science products for several agency and national projects and initiatives.

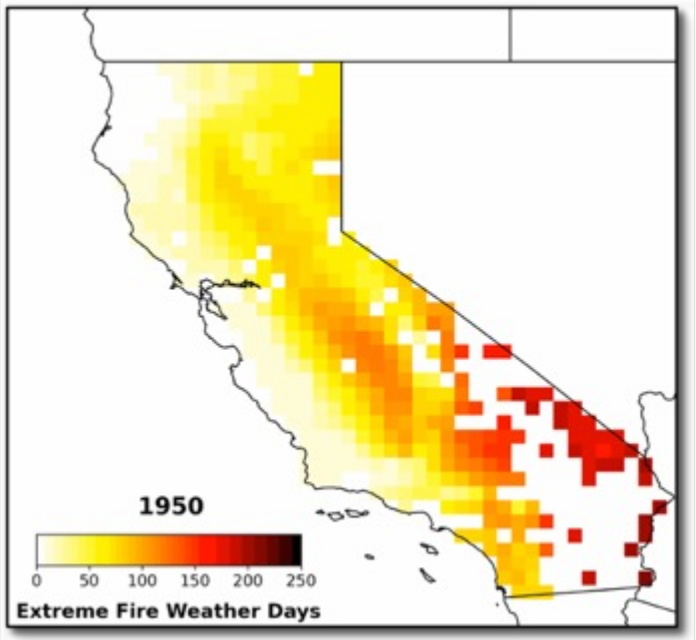
Key Results

- Supported GeoNEX activity for NASA's Short-term Prediction Research and Transition Center GEO-Kompsat 2A weather satellite, automated data management and acquisition; and implemented the GeoNEX surface downwelling solar radiation algorithm and generated DSR products.
- Completed reprocessing of the Hyperion EO-1 satellite dataset and generated Ames Global Hyperspectral Synthetic Dataset in support of the Surface Biology and Geology (SBG) mission, a NASA Earth System Observatory core mission that successfully completed a Key Decision Point review in 2022.

Role of HECC

- The NASA Advanced Supercomputing facility's supercomputers, networks, and storage systems, including NEX-dedicated filesystems, are all available at no cost to NEX users. GeoNEX and SBG products are made publicly available via the NAS Data Portal—crucial for the NEX goal of facilitating Earth science in the wider community.

BENEFIT: NEX participates in the development of the Surface Biology and Geology mission, which is directly responsive to the 2017 Earth Decadal Survey, and supports the National Climate Assessment. GeoNEX activities address NASA's strategic vision to protect and improve life on Earth.



"Our relationship with HECC has enabled us to conduct cutting-edge research and development in support of NASA's Earth Science Division." *— Ian Brosnan, NASA Ames*

Investigating the Orbits, Sizes, and Impact Rate of NEOs

Summary

- Understanding the Near-Earth-Object (NEO) population is important for planetary defense. At the request of NASA's Planetary Defense Coordination Office, scientists at Southwest Research Institute (SWRI) successfully developed a new orbital model of NEOs by numerically integrating asteroid orbits from main belt sources and calibrating the results on observations of the Catalina Sky Survey. Results will be used for mission planning and a means to gauge progress toward the NEO search goals.

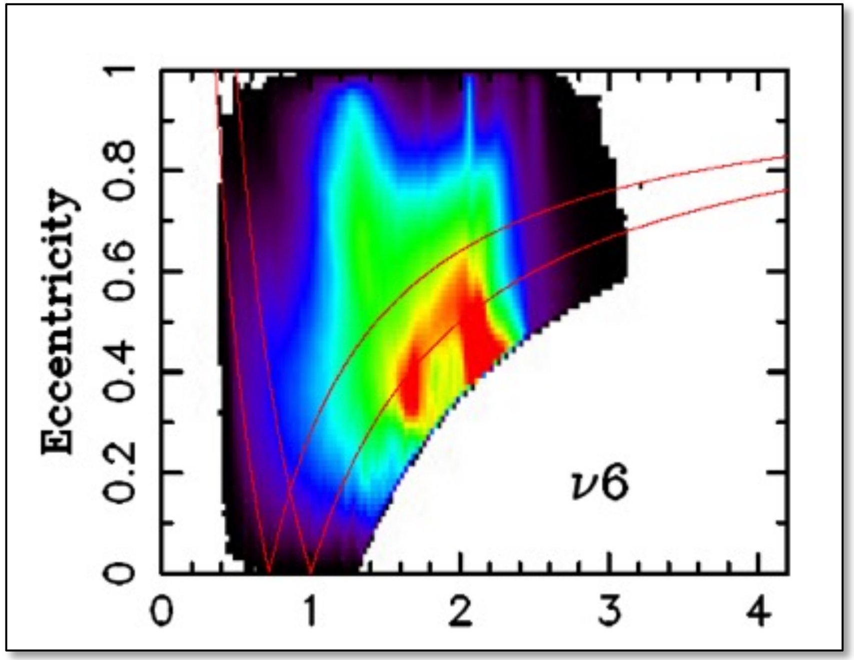
Key Results

- The SWRI team found that most multi-kilometer NEOs come from the central/outer asteroid belt, while most sub-kilometer NEOs come from the inner asteroid belt. They confirmed that NEOs disrupt near the Sun, and that the disruption process is size dependent.
- The team also confirmed that asteroids need to drift at predicted rates across the asteroid belt by the Yarkovsky effect to keep the NEO population in steady state. Their work also included calculating the NEO impact rate for Earth, Moon, and the other terrestrial planets.

Role of HECC

- Numerical integration simulations tracking asteroid orbits forward in time were performed on 2,000 Pleaides Ivy Bridge nodes, representing a total of 10 million CPU hours. Parallel processing on Pleiades enabled the team to come up with "fits" between their multi-source model and data.

BENEFIT: This work will benefit the upcoming NASA NEO Surveyor mission, a space-based infrared survey scheduled to launch in 2027, with a goal to search for threatening NEOs that are larger than 140 meters in diameter.



"The work on our NEO model could not have been accomplished without HECC resources, as we lacked the computational resources at our home institution to do this work."

— William Bottke, Southwest Research Institute

Investigations into Mercury's Dynamic Magnetosphere

Summary

- Using data from NASA's MESSENGER mission, researchers at Princeton University investigated the myriad roles of key kinetic and multifluid effects in Mercury's magnetospheric responses to solar wind drivers, including extreme space weather events. The team applied a 3D multifluid magnetohydro-dynamic (MHD) model and the kinetic Magnetohydrodynamic with Adaptively Embedded Particle-In-Cell model to simulate the generation, circulation, and distribution of sodium ions; in addition to the dawn-dusk asymmetry of Mercury's magnetotail current sheet and the reconnection onset.

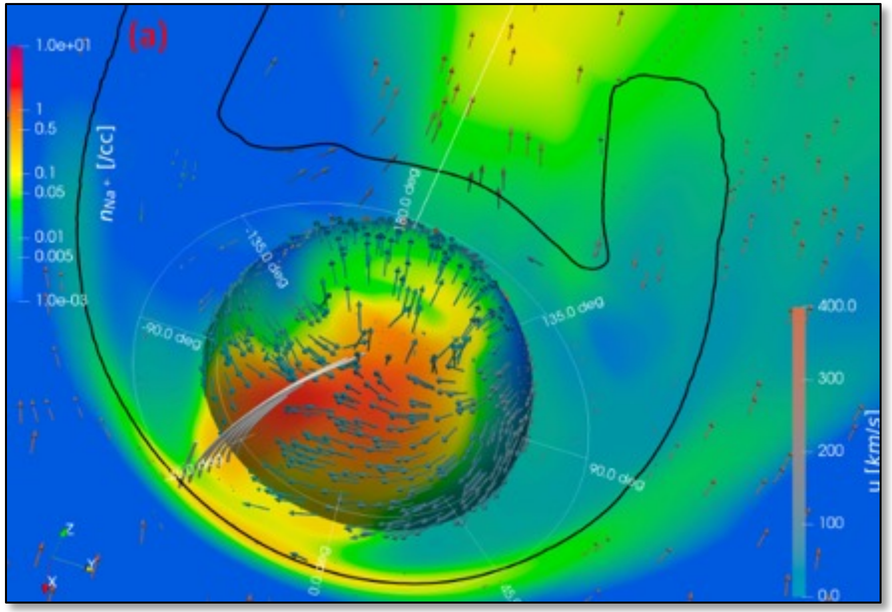
Key Results

- Results show that the asymmetric plasma distributions and magnetospheric convection pattern arise from the flow velocity separation between the sodium fluid and solar wind fluid. The simulations also show that a non-ideal MHD effect causes the asymmetries of magnetotail reconnection, and explain why the magnetic flux ropes and high-speed electron jets are more frequently observed by MESSENGER on the dawnside.

Role of HECC

- Using 25,600 cores on Pleiades, the team launched 100 billion macro-particles in their particle-in-cell code to investigate the kinetic effects on Mercury's magnetospheric dynamics, which produces terabytes of output.

BENEFIT: These simulations directly address the scientific objective to investigate the role of planetary heavy ions in Mercury's magnetosphere and provide a new mechanism to explain the asymmetric ion distributions that have been observed by NASA's MESSENGER mission.



"HECC provides stable and user-friendly computational and storage resources for performing global-scale kinetic magnetospheric simulations. Without the stable IO system, we would have been unable to successfully complete the simulations." — *Chuanfei Dong, Princeton University*

Run on Request Service for Space Weather Modeling

Summary

- The Community Coordinated Modeling Center (CCMC), located at NASA Goddard, is a multi-agency partnership to enable, support, and perform research and development for next-generation space science and space weather models. CCMC hosts a unique and expanding collection of models developed by the international research community and provides associated services to any researchers interested in running and evaluating those models. Run on Request (ROR) is a CCMC service where customers can request a space weather model simulation and receive results through a web page.

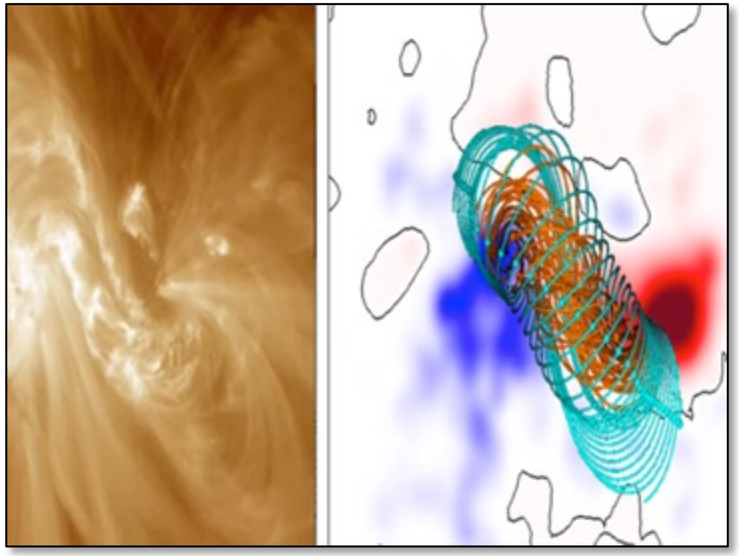
Key Results

- ROR staff often use HECC resources to perform model runs. In FY22, CCMC and its partners onboarded and/or evaluated four additional models: Whole Atmosphere Community Climate Model with thermosphere and ionosphere extension; Data Assimilation Research Testbed - Thermosphere Ionosphere Electrodynamics General Circulation Model; HYbrid Particle Event-Resolving Simulator: Global 3D; and Grid Agnostic MHD for Extended Research Applications.

Role of HECC

- HECC resources and services supplement CCMC's resources and allow computationally expensive simulations that could not be done on premises. HECC services are performed in a timely and transparent manner, without the barriers of setting up and maintaining expanded HPC infrastructure.

BENEFITS: The Run on Request service at the CCMC permits expert and novice scientists across the world to exercise state-of-the-art space weather models in order to help NASA and its partners better understand and predict the impacts of space weather events on aerospace assets, in support of robotic and human exploration missions.



"HECC supercomputers enabled CCMC to shorten simulation services turnaround times that could have taken longer with our own systems. The simulations allow U.S. and international researchers to research, validate and demonstrate their results in scientific or educational presentations."

— Tina Tsui, NASA Goddard

Evaluating the GEOS Climate Chemistry Model

Summary

- As part of the agency's efforts to improve the accuracy of global climate model predictions, researchers at NASA's Goddard are quantifying the equilibrium climate sensitivity (ECS) of the Goddard Earth Observing System's (GEOS) Chemistry Climate Model (CCM), providing insight on whether GEOS can be used as a climate model when run coupled to chemistry configurations.

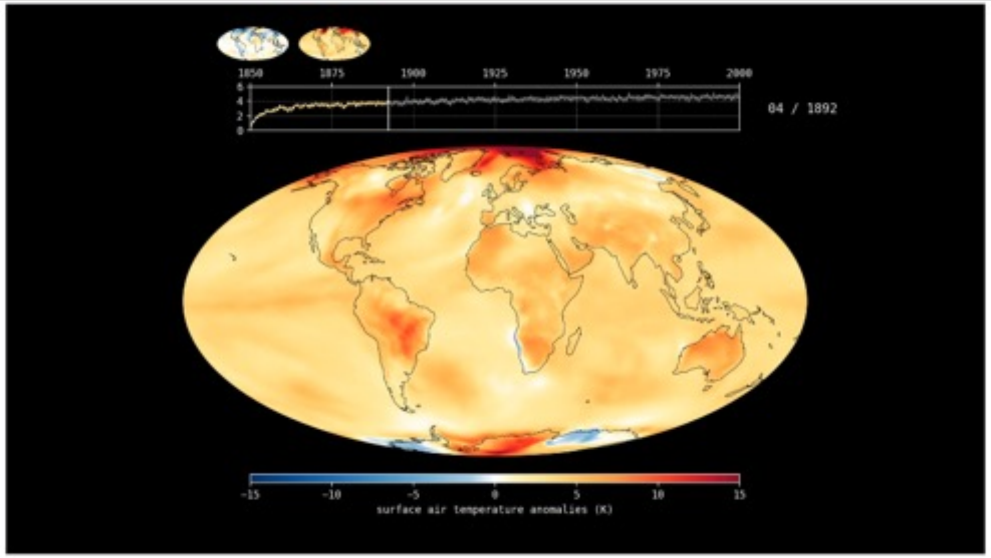
Key Results

- The team ran a pair of long simulations with the GEOS coupled ocean-atmosphere model: a pre-industrial control simulation using 1850 conditions run for 150 years, assuming fixed CO_2 abundance and emissions; and a variation that instantly quadruples the abundance of CO_2 started from the endpoint of the pre-industrial control. The two simulations are used to calculate ECS of the model, which, in addition to other diagnostics computed from the simulations, showed that the GEOS CCM is well within the range of previously evaluated models.

Role of HECC

- The simulations used almost twenty 40-core CPUs each, which allowed the team to run a year of simulated model time in a little over a day. It would have taken almost twenty years of real-world time on a typical desktop to run the 300 years simulated as part of this project, while the team was able to achieve their results on Pleiades in around six months.

BENEFIT: This effort is foundational to future climate prediction work with the GEOS CCM by establishing the basic credibility of the coupled atmosphere-ocean model for simulating climate change. Future work will introduce detailed chemistry mechanisms and impose time-varying changes to emissions to more realistically produce changes in ozone.



"The high-performance computing resources at the NASA Advanced Supercomputing facility, particularly the Pleiades supercomputer, are essential to carrying out this work."
— Katherine Knowland, NASA Goddard

Simulating Accretion Disk Eccentricity in Dwarf Binaries

Summary

- Researchers at the Flatiron Institute and the University of California Santa Barbara used radiation magnetohydrodynamic (MHD) codes run on HECC systems to conduct global simulations of the most compact accretion white dwarf binaries in nature: AM Canum Venaticorum (AM CVn) star systems, where a white dwarf accretion disk is being fed by a helium donor star. Their work investigates how disk eccentricity is developed with self-consistent magnetorotational instability (MRI) turbulence and how it might explain the observed variability by NASA missions like Kepler and TESS.

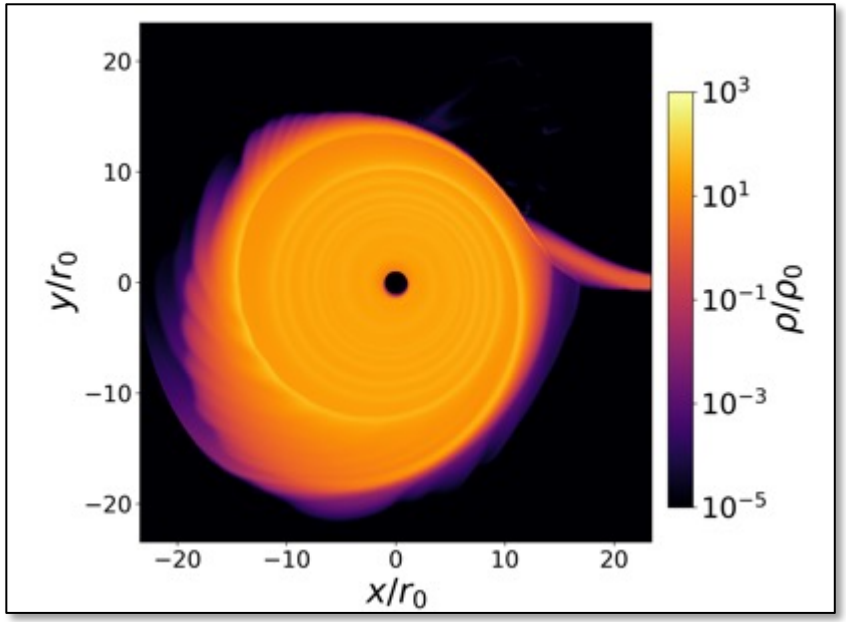
Key Results

- The team successfully reproduced the development of eccentricity in the AM CVn system with hydrodynamic simulations. They performed a series of MHD simulations with different magnetic field strength so that MRI turbulence could drive disk accretion self-consistently without artificial alpha viscosity. Results showed the dominant term contributing to eccentricity growth is the tidal gravity of the companion star, and that MRI turbulence does not saturate at a high enough state to reproduce the observed superhumps in 3D MHD simulations.

Role of HECC

- Properly resolving the MRI turbulence in the compact binary system requires a few thousand CPUs for each simulation. The development of eccentricity in the model also requires hundreds of binary orbits, which means each simulation needs to run for a long time.

BENEFIT: This work provides a reliable test of magnetorotational instability turbulence based on superhump phenomena observed by NASA's Kepler missions, and the results have a wide range of implications for our understanding of this phenomena and its application to other accretion system studies.



"The HECC resource is the only computational cluster that we can use for this project. It makes it possible for us to perform these calculations."
— Yan-Fei Jiang, Flatiron Institute

Modeling the Interior Dynamos of Jupiter and Saturn

Summary

- Researchers at Harvard University are using simulations run on HECC systems to better understand the internal dynamo mechanisms inside Jupiter and Saturn. Their goal is to produce models that can match magnetic field measurements by NASA's Juno and Cassini missions to reconcile our theoretical understanding of the planets' complex dynamos with observations.

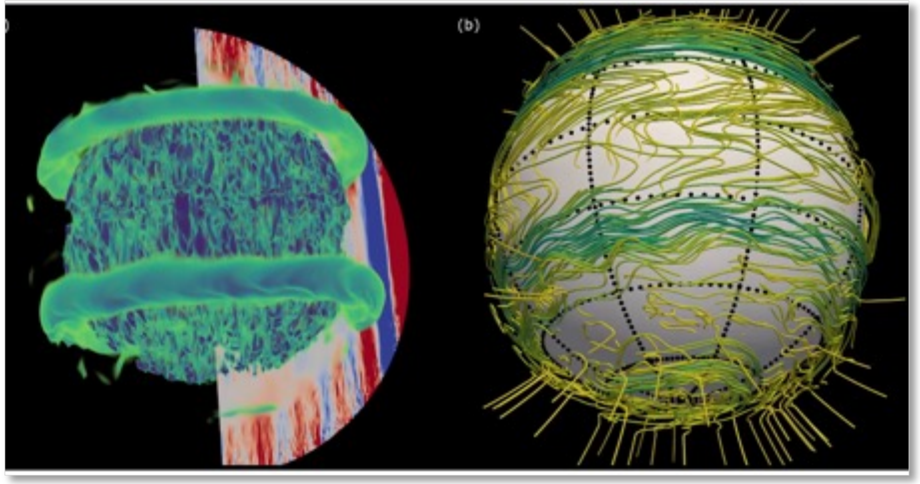
Key Results

- Using the 3D magnetohydrodynamics code MagIC, they ran new cases for Jupiter's dynamo, altering parameters from earlier promising simulations to test stability. They found that the new simulations maintain their dipole dominant magnetic fields, but the field geometry lacked close similarity to observations. Future work will investigate these discrepancies.
- To understand the dynamics of Saturn's interior and atmosphere, they developed a dynamo simulation that was able to successfully produce fluid dynamics phenomena seen in Saturn simultaneously, like jet streams, cyclonic and anticyclonic vortices, and a dipole-dominant, axisymmetric magnetic field.

Role of HECC

- The high-fidelity supercomputer simulations for the Saturn and Jupiter dynamo projects use first-principle fluid dynamics to mimic the complex processes in the planets' surface and interior, bringing us one step closer to understanding their inner workings.

BENEFIT: These studies aim to improve our understanding of the data collected by the Cassini and Juno spacecraft to Saturn and Jupiter. This is achieved through the development of highly accurate numerical models, which shed light on the complex fluid dynamics observed by the spacecraft. Ultimately, the projects seek to increase our knowledge of the origins and evolution of these planets.



"The resources provided by HECC are nothing less than a life line for the Jupiter dynamo project. The high level of turbulence involved in the simulations, as well as the multilayer approach we take in designing the grid, demands very high resolution. Such high-fidelity simulations simply cannot be simulated elsewhere."

— Rakesh Yadav, Harvard University

Exploring Wave Generation in the Solar Wind and Corona

Summary

- In an effort to meet the goals of the Laboratory Nuclear, Atomic, and Plasma Physics heliophysics program, investigators from the Space Science Institute used high-performance computing resources to study how electron beams propagating through background plasma generate waves. High-fidelity kinetic simulations run on HECC supercomputers were also compared to dedicated experiments performed in UCLA's Large Plasma Device.

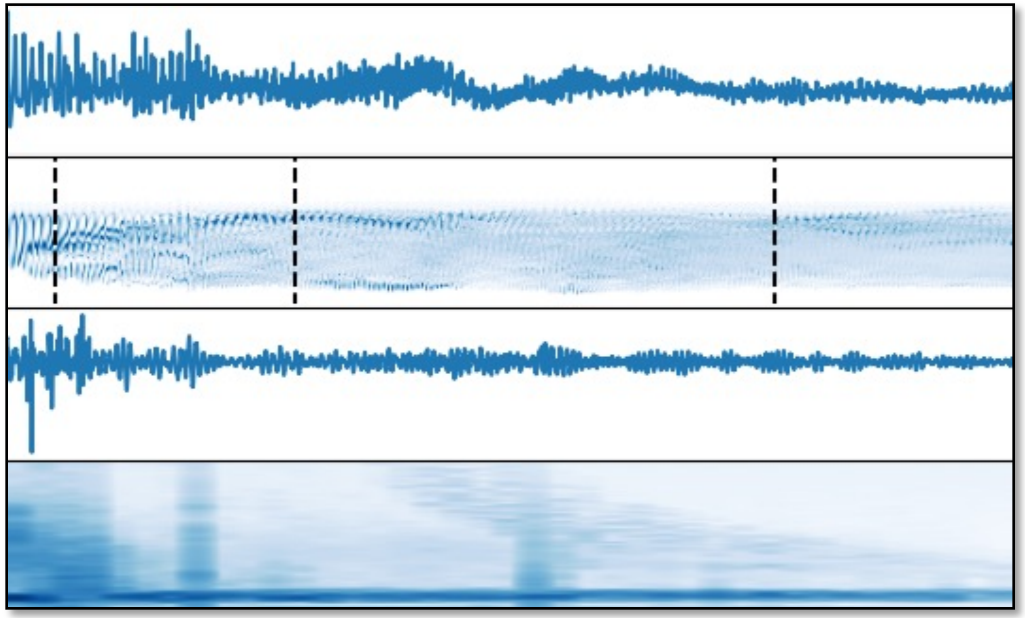
Key Results

- In the last year, the team significantly improved the realism of the simulations. In particular, simulations were performed at lower values of plasma pressure than previously possible. Such simulations are more computationally challenging, but necessary for successful comparison with the UCLA experiment. Using these new models, the team studied mechanisms producing "clumpy" or "bursty" Langmuir wave packets observed in experiments. Similar phenomena are also often observed in the solar wind and in the auroral ionosphere. Comparing simulations to the experiment and the spacecraft data helps understand nonlinear processes at work.

Role of HECC

- This project required computationally expensive, high-resolution simulations that are essential to interpretation of observational measurements, including spacecraft data where measurements are necessarily limited in coverage.

BENEFIT: This research provides a new understanding of physical processes directly relevant to NASA's heliophysics goals to study the impact of the Sun on the Earth and solar system, and to develop technology to detect and predict extreme conditions in space. The results of the investigation will impact the Parker Solar Probe mission by providing a deeper understanding of observational data.



"The large-scale computational resources provided by HECC are essential to enable success of the overall project."
— Vadim Roytershteyn, Space Science Institute

Tackling the Physics of Black Holes in Massive Disks

Summary

- Researchers at the University of Illinois at Urbana-Champaign are using HECC supercomputing resources to simulate highly spinning supermassive black holes in magnetized self-gravitating massive disks, merging black hole-neutron star binaries, and dwarf-neutron star binaries of various mass ratios. These complex models are used to model gravitational waves and to explain some electromagnetic signals that can be detected by current NASA spacecraft, as well as to gain a better understanding of these observations and the physics of matter under extreme conditions.

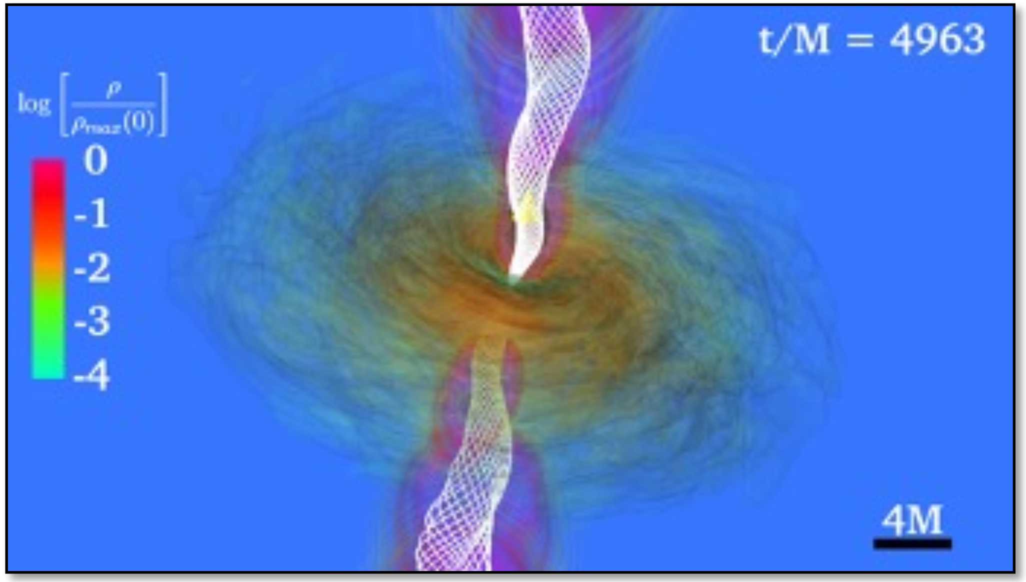
Key Results

- Using their in-house GRMHD code for running state-of-the-art, high-resolution, shock-capturing simulations on HECC systems, the team accurately computed initial sequences black hole-disk systems ranging from massless to really heavy massive disks. They were able to extend these calculations to incorporate highly spinning black holes (almost extremal spinning), and were able to clarify the role of different general relativistic spin measures.

Role of HECC

- The team has noticed that their codes perform better on HECC supercomputers (particularly Pleiades) than on other clusters. On Pleiades, they observe perfect scaling up to 64 nodes and around 85% scaling to 128 nodes, compared to around 80% scaling on 64 nodes on the Blue Waters (NCSA) and Stampede (TACC) systems.

BENEFIT: Galactic simulations of black holes in massive disks such as the ones performed for this work not only advance our understanding of these phenomena, but help to analyze and understand signals and observational data gathered by agency spacecraft.



"Our effort to tackle several large-scale, long-standing, unsolved problems in theoretical astrophysics depends on the resources provided by HECC. Running and analyzing our long-term simulations require a large allocation, which is extremely limited at other supercomputer centers."

— Milton Ruiz, University of Illinois at Urbana-Champaign

Simulating Gravity Fields for Cislunar Operations

Summary

- Researchers at NASA JPL are utilizing HECC computational resources to develop the highest resolution lunar gravity field model available to date, which uses the latest lunar ephemeris and rotational model (DE440) for future cislunar operations. This is part of a nearly 60-year goal of the agency to better understand the Moon's gravity field to ensure accurate navigation and landing for lunar missions.

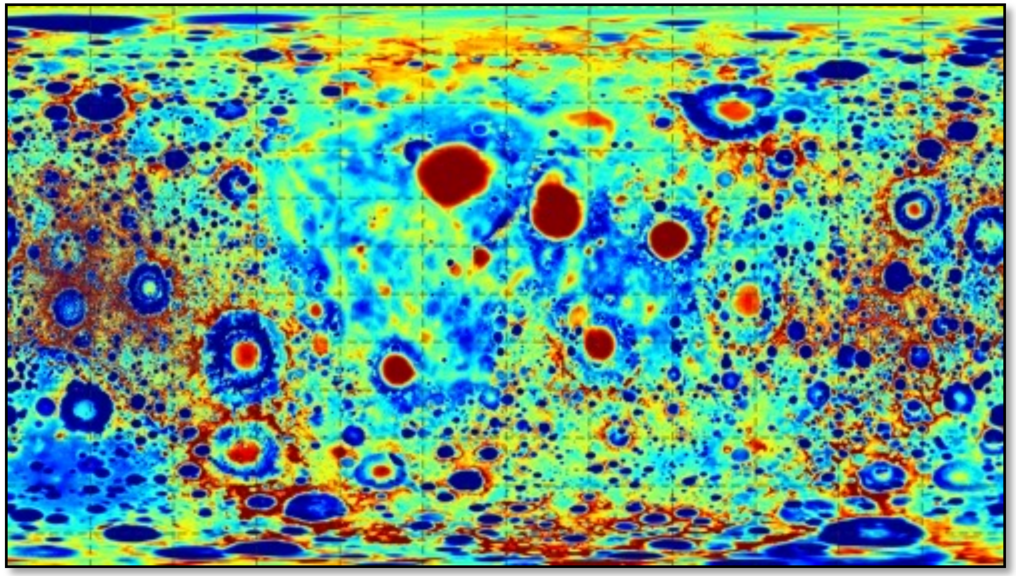
Key Results

- Using JPL's MIRAGE software, the team used data gathered by lunar satellites, such as the Gravity Recovery and Interior Laboratory (GRAIL) and Lunar Prospector missions to solve for a significantly higher harmonic gravity field than previous efforts. Over the last decade, this has resulted in new discoveries about the lunar interior from crust to core, and improved lunar orbit determinations for current satellite missions. Processing of data from GRAIL's lower-altitude extended mission has doubled the resolution of the gravity field model, leading to further science discoveries and navigation improvements. A few more solutions are needed to complete the project by FY23.

Role of HECC

- The estimation process of determining the highest resolution lunar gravity field requires multiple summations and inversions of a matrix of around 40 terabytes. With multiple solutions needed to assess error statistics, HECC resources have been critical to computing these high-resolution simulations.

BENEFIT: Understanding the gravity field of the Moon allows for precision spacecraft navigation and provides insights into cislunar space—the region from the Earth to the surface of the Moon—and the lunar interior structure and geophysical processes.



"The primary goal of our project is to deliver a high-resolution lunar gravity field that is tied to JPL's latest-available lunar rotational model, DE440. This task needs to simultaneously estimate over 3 million parameters, requiring HECC resources."

— Ryan Park, NASA JPL

Developing Algorithms and Tools for the SWOT Mission

Summary

- Before the Surface Water and Ocean Topography (SWOT) mission launched in January 2023, its system engineering team based at NASA JPL ran simulations on HECC systems to prepare for the mission's commissioning phase during the first three months after launch.
- During its mission, SWOT's primary instrument, the Ka-band Radar Interferometer (KaRin), will continuously collect data over the ocean. To maintain the data volume at a reasonable level, the radar includes a sophisticated on-board processing (OBP) algorithm.

Key Results

- The JPL team generated many simulations of possible scenarios that may occur during the mission to help develop and validate the OPB algorithm and other software tools used in SWOT's commissioning phase to set the correct radar parameters that will ensure valid data will be collected during the mission. These tools are now ready to go for the mission phase.

Role of HECC

- The computationally intensive SWOT radar data simulations require the enormous amounts of compute capability and memory storage provided by the Pleiades and Electra supercomputers in order to complete in a timely manner. By enabling the team to develop and validate their algorithms and tools, HECC is an essential element for the success of this mission.

BENEFIT: Testing the algorithms to be used in the SWOT mission is essential for its success. The mission, which will provide new data for physical oceanography and hydrology communities, was recommended to NASA by the National Research Council's decadal review "Earth Science and Applications from Space: National Imperatives for the Next Decade and Beyond."

"HECC is an indispensable resource that enabled us to develop the tools required in SWOT's commissioning phase. — *Samuel Chan, NASA JPL*

TESS Science Processing Operations Center Pipeline

Summary

- As a critical element of the NASA Explorer Program's Transiting Exoplanet Survey Satellite (TESS) Mission, the Science Processing Operations Center (SPOC) operates as the official pipeline of record. Each month, the SPOC processes the raw image data acquired by TESS to produce calibrated data, light curves, and transiting planet search products and reports for 20,000 |two-minute target postage stamp data, and calibrated pixels and light curves for about 1,600 twenty-second target star postage stamp data.

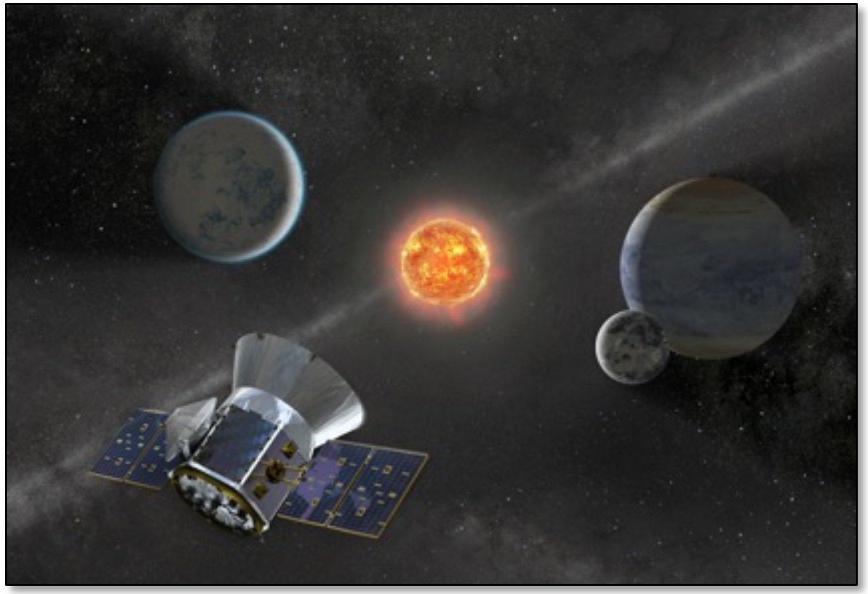
Key Results

- In the past year, the SPOC identified 50,763 (non-unique) potential transiting exoplanet signatures and associated diagnostics to the TESS Science Office, which released 300 new TESS Objects of Interest from the SPOC pipeline. As of April 18, 2023, there were 329 confirmed planets with 6,400 candidate planets. TESS exoplanets represent the majority of the targets to be followed up and characterized with the James Webb Space Telescope.

Role of HECC

- Not only does the SPOC team use the Pleaides supercomputer for several processing steps, HECC also maintains the SPOC servers and filesystem within the secure enclave. The pipeline's Photometric Analysis, Transiting Planet Search, and Data Validation modules run on HECC systems across thousands of CPUs. Multi-sector and multi-year transit searches rely on HECC to store hundreds of terabytes spanning the entire TESS mission.

BENEFIT: NASA's Science Processing Operations Center directly supported the TESS mission's achievement of the Level 1 Science Requirement to discover at least 50 planets smaller than Neptune for which mass measurements are obtained. TESS has discovered and measured the masses of over 100 planets smaller than 2.5 Earth radii, greatly exceeding the Level 1 requirement.



"The TESS mission could not succeed without NASA HPC resources. The enormous computational power provided by the HECC systems is a key enabling technology for TESS." ***— Eric Ting, NASA Ames***

Modeling Dynamical Processes in the Solar Interior

Summary

- Researchers at the University of Colorado Boulder ran 3D global simulations to better understand the dynamical processes within the solar interior, focusing on the dynamics within the convection zone-radiative zone interface where the tachocline resides. The team aims to create a self-consistent, fully nonlinear model of the tachocline dynamics and assess the role and importance of a tachocline for the solar dynamo process.

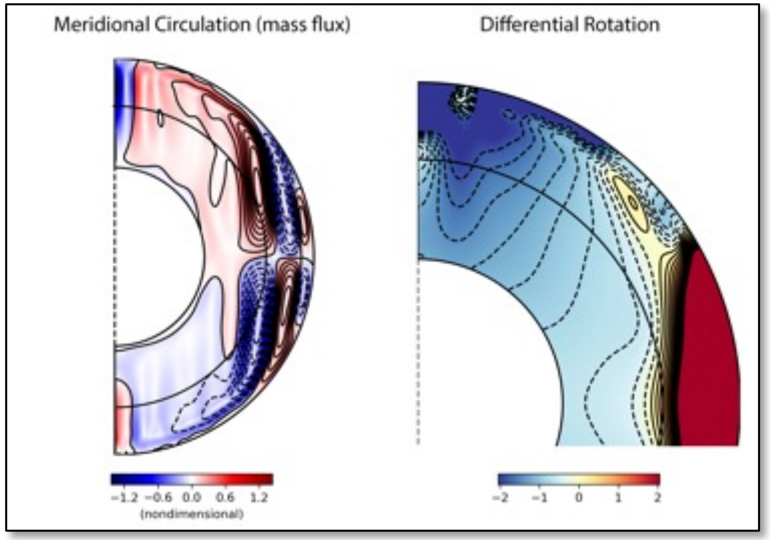
Key Results

- The team performed a systematic study via the use of numerical simulations that spanned a wide parameter space. They identified which parameter regimes lead to a solar-like differential rotational profile with the equatorial region rotating faster than the poles and with non-cylindrical contours at mid-latitudes in the convection zone.
- Within the simulated solar-like parameter regime, they found that the meridional flows which arise due to rotation can penetrate below the base of the convection zone, deeper into the stable layer, and that the viscous stresses do not play an important role in the angular momentum transport—an observation similar to what researchers expect is occurring in the Sun.

Role of HECC

- Most of the 30 models developed in this study possessed a spatial resolution of at least 192×528×1056 and required many months to run using approximately 4,100 Pleiades Broadwell cores.

BENEFIT: This work addresses a fundamental challenge in heliophysics—to understand the dynamics driving the Sun's magnetic activity cycle—supporting NASA's heliophysics strategic objective "to understand the Sun and its interactions with Earth and the solar system, including space weather."



"The resources required to evolve our models are far beyond those available on a modern desktop or a typical university cluster. These simulations are necessary for gaining a better understanding of the complicated dynamics occurring in the solar interior and would not be possible without HECC resources." — Lydia Korre, University of Colorado Boulder

N_2O IR Spectral Data for Exoplanet Atmosphere Modeling

Summary

- Researchers at NASA Ames are using the Aitken supercomputer to construct an accurate infrared (IR) spectral database for nitrous oxide (N_2O) to characterize astrophysical environments containing N_2O—one of the most important potential biosignature molecules in exoplanets that reside in habitable zones.

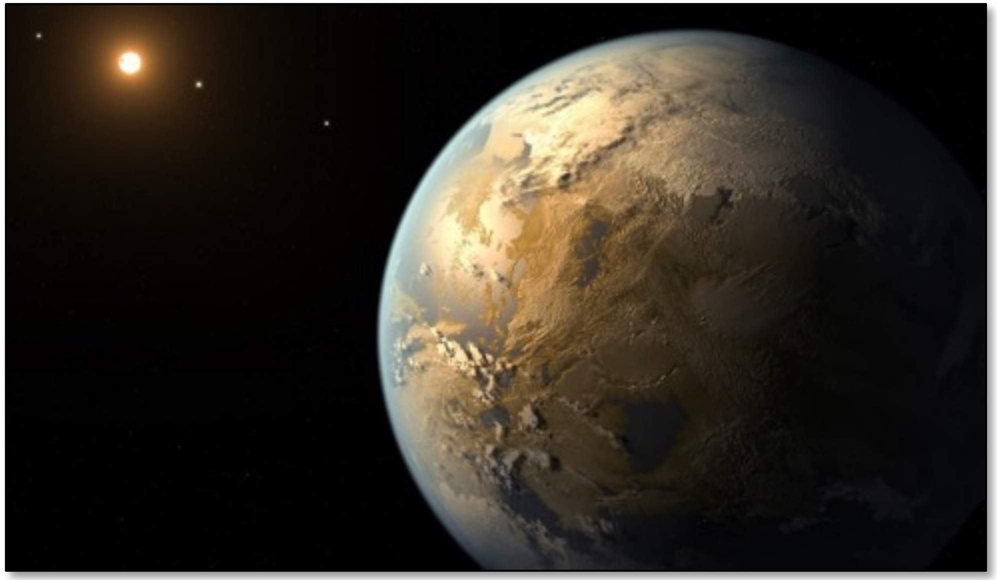
Key Results

- The team computed highly accurate IR line lists at 296 Kelvin for the six most abundant N_2O isotopologues. Compared to recent experiments, the line lists provide much more complete coverage as well more reliable and consistent predictions for those bands missing from current databases.
- The spectral library and other data products are made available to the astrophysical and space science communities, facilitating the chemical diagnostics of exoplanet and dwarf atmospheres, as well as their physical conditions. They will also be published with open access to the public.

Role of HECC

- This work was made possible by the large shared memory available on Aitken's Rome nodes. The memory also functions as a virtual hard drive with very fast I/O, which provided significant advantages in computing the nitrous oxide line list as well as performing various tests and evaluations.

BENEFIT: The results of this work will enable the N_2O spectral analysis and opacity simulation required to enhance the scientific return from astronomical observations of NASA missions such as the Stratospheric Observatory for Infrared Astronomy (SOFIA), James Webb Space Telescope, and the upcoming Nancy Grace Roman Space Telescope.



"The whole N_2O project is computer resource intensive. The success of our project and its achievements fully relied on the HECC resources allocated to us in FY22."

— Xinchuan Huang, NASA Ames

Characterization of Stellar Jitter Using 3D Realistic Models

Summary

- To enhance the agency's capabilities to detect Earth-size planets, scientists at NASA Ames developed 3D realistic radiative hydrodynamics models of solar-type stars to characterize and understand the nature of "stellar jitter," the photospheric noise produced by planet-host stars. Understanding the properties and sources of stellar jitter will enable techniques to achieve 10-centimeters-per second accuracy of the radial velocity measurements.

Key Results

- The team developed a data postprocessing and analysis pipeline to obtain a time series of synthetic observations of target stars; this enables them to understand how center-to-limb effects, structure, and dynamics of the photosphere contribute to the disk-integrated signal on observations.
- Using their in-house StellarBox code, they developed stellar models of several planet-host stars and generated a time series of synthetic spectra with ultra-high resolution. This approach demonstrates the agency's capability to capture various known effects and reveal the impact of nonhomogeneous atmospheric flows on systematic variations of the disk-integrated observations.

Role of HECC

- HECC resources provided a unique opportunity to disentangle the photospheric noise contribution and contribute to the community effort to detect the radial velocity variations induced by Earth-mass planetary motion.

BENEFIT: These models are crucial to understanding the physics of turbulent surface disturbances that contaminate planetary signals in observations. The models can be used to develop new approaches to characterize stellar surface effects, help interpret ground and space observations, and improve the detection rate of Earth-type planets.

"Our models, enabled by HECC resources, allow the development of a new generation of physics-driven methods to achieve extreme precision of radial velocity to detect Earth-mass exoplanets."
— Irina Kitiashvili, NASA Ames

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