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AERONAUTICS (ARMD)

Demo 1

A Breakthrough in Rotorcraft Prediction Accuracy Using Detached Eddy Simulation

Overview

Helicopters and tiltrotors provide many useful civil and military functions without the need for airports and runways. Modern rotorcraft designs continue to push the technology to improve vehicle performance, safety, and reduce its impact on the environment. However, the accurate simulation of rotorcraft flow fields with computational fluid dynamics (CFD) continues to be a challenging problem. Rotor blades generate blade-tip vortices as they spin around and encounter the vortices of other blades as well. This can result in very complex blade vortex interaction (BVI) and vortex wake interactions. Moreover, rotorcraft simulation is multidisciplinary and must take into account the interaction between rotor blade aerodynamics, blade flexibility, and blade motions to achieve trimmed steady flight.

Project Details

The figure of merit (FM), the chief hover performance parameter, is under predicted by 2-6% depending on the numerical approach. To bring this into perspective, every ½% error means there is one less passenger the vehicle can carry. Moreover, under resolved rotor wakes result in inaccurate interactions between the rotor vortices and the rest of the vehicle. One goal of NASA's Rotary Wing (RW) Project is to develop physics-based computational tools to improve the predictive accuracy of these flow fields. The OVERFLOW CFD code is used to solve the time-dependent Navier-Stokes equations for the V22 Osprey tiltrotor and UH-60 Blackhawk helicopter rotors in hover and forward flight.

Results and Impact

The FM has been predicted within experimental error for the first time for the V22 Osprey and Blackhawk helicopter rotors in hover over a wide range of flow conditions. This dramatic improvement is due to the use of algorithms with high-order spatial accuracy, refined grid resolution on the rotor blades, and an improved detached eddy simulation (DES) hybrid turbulence model. High resolution accuracy on the rotor blades was important for all cases studied, but the DES hybrid turbulence model was crucial in BVI cases.

Dynamic adaptive mesh refinement (AMR) is used to efficiently resolve the rotor wakes. This is accomplished by detecting vortices and locally added blocks of Cartesian grids of higher resolution. This allows the vortices and rotor wake to be resolved by grids four times finer and at half the computational cost than a uniform (non AMR) grid refinement approach. The AMR resolution revealed tremendous detail of the blade vortices and turbulent flow that had never before been observed computationally or experimentally. The flow simulations have been quantitatively validated with experimental measurements.

The use of AMR greatly improved the prediction of vortex core size and growth with wake age (distance along the tip vortex). The error in vortex core growth rate has been reduced from 60% to 4% error.

These groundbreaking results will impact the next generation of rotorcraft analysis and design.

Role of High-End Computing Resources and Services

These flow simulations were made possible by NASA's Pleiades supercomputer. Solutions typically required 1,500-4,600 cores for 1-2 weeks. Grid sizes varied from 60-750 million grid points, and required 5-24 hours of wall time per rotor revolution.

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Demo 2

Adjoint-Based Design for Complex Aerospace Configurations

Overview

This effort seeks to enable formal constrained design optimization of complex aerospace configurations experiencing unsteady turbulent flows and requiring dynamic/deforming geometries and high-fidelity physical models. Since a single simulation of this type may require millions of compute hours, highly efficient strategies must be developed to compute accurate sensitivities for many thousands of design parameters. Adjoint-based methods implemented on massively parallel computing architectures allow the designer to formally tackle a broad range of complex optimization problems across the speed range which would otherwise remain computationally intractable. The overall approach is implemented in the NASA Langley FUN3D solver

Project Details

In a typical fluid dynamics problem, the governing equations are integrated forward in physical time to determine aerodynamic quantities of interest. To efficiently compute sensitivities of these quantities with respect to thousands of input parameters, the adjoint approach solves the linearized governing equations in reverse physical time. In this manner, the adjoint solution marches backwards in time to determine the sensitivities of output functions due to any input parameters required for the simulation.

A discrete adjoint approach is taken in which the discretized governing equations are linearized exactly with respect to the flowfield and mesh variables. The implementation supports steady and unsteady flows based on compressible and incompressible forms of the Reynolds-averaged Navier-Stokes equations. Computational meshes may include general element types belonging to single block or overset grid topologies. Furthermore, these grids may be rigidly moving, deforming, or any combination thereof; general parent-child body motion relationships are also accommodated.

Results and Impact

The effort required to develop and mature this general capability has taken two decades of sustained research and software development. The approach has been successfully

demonstrated on a broad range of realistic design problems, including rotorcraft geometries, fighter jets, biologically-inspired micro air vehicle configurations, active flow control systems, and wind energy devices. The adjoint-based methodology also provides a rigorous foundation, valuable insight, and an effective tool for error estimation, mesh adaptation, and uncertainty quantification for such problems.

Role of High-End Computing Resources and Services

A relatively simple single-point design optimization typically requires the equivalent cost of $O(30)$ flow simulations. Since a single simulation for this class of flows may require millions of compute hours, efficiently exploiting the world's most powerful supercomputing systems is essential. Furthermore, solution of the adjoint equations requires that the complete forward solution be available during the reverse integration in time. This translates to terabytes of data I/O for even moderately-sized problems; development of a highly efficient asynchronous parallel I/O strategy has been an enabling element of this work.

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Demo 3

Simulating Hypersonic Turbulent Combustion for Future Aircraft

Overview

Future access-to-space activities and transoceanic air travel may rely on advanced aero-propulsion concepts to enable hypersonic flight (Mach numbers greater than 5). A hydrogen-fueled scramjet (supersonic combustor ramjet) is one type of engine capable of hypersonic flight, and the analysis, design, and optimization of such engines relies heavily on computational fluid dynamics. A more accurate way of computing the reactive flow within scramjet engines is through large-eddy simulation (LES), which directly calculates the larger turbulent eddies responsible for mixing of fuel and air. In this work, we conduct LES simulations of the reacting flow within a model scramjet tested at the University of Virginia.

Project Details

For this project, we solve the compressible Navier-Stokes equations governing a reacting mixture of gases using a large-eddy simulation strategy. Finite-rate hydrogen-air combustion is modeled through a nine-species / nineteen reaction mechanism. The equations are advanced in time using an implicit method. Low-dissipation discretization schemes are used to allow resolution of small turbulent eddies. The calculations use meshes ranging size from 35 to 70 million cells and were performed using NCSU's REACTMB flow solver. Results were compared with experimental data collected at the University of Virginia.

Results and Impact

Our research shows that flame stabilization in the University of Virginia's model scramjet combustor is a complex process, dependent on the interplay between the relatively fast

hydrogen oxidation kinetics, high mixing rates induced by the flameholder geometry, and flame stretch effects induced by large-eddy interaction with the flame surface. The LES methodology provides much better predictive capability, compared with Reynolds-averaged Navier-Stokes methods that are in popular use. Excellent agreement with experimental temperature, mole fraction, velocity, and pressure measurements have been obtained.

Role of High-End Computing Resources and Services

These simulations simultaneously solve upwards of 500 million equations and have been performed on hundreds of processors simultaneously on NASA's Pleiades supercomputer. Each simulation requires several days to complete and generates from 4 to 8 terabytes of data.

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Demo 4

From a Roar to a Whisper: Making Modern Aircraft Quieter

Overview

Aircraft noise is an environmental hazard that affects metropolitan areas adjacent to major airports. With the projected growth in air travel, the noise exposure levels are expected to increase substantially. The Environmentally Responsible Aviation (ERA) project of the NASA Aeronautics Mission Research Directorate is developing and maturing noise reduction technologies that will confine aircraft noise footprints on the ground within airport boundaries. This is to be accomplished without detrimental effects to the aerodynamic efficiency of aircraft.

To most people, aircraft noise is synonymous with jet engine noise. During approach to landing, however, noise generated by the airframe is comparable to, and in some instances even louder than, propulsion noise. The prominent sources of airframe noise are the landing gear and lift generating devices such as wing flaps and slats.

Project Details

As part of the ERA-Gulfstream partnership on airframe noise research, we simulated the airflow over a semi-span model of a Gulfstream aircraft in landing configuration. We focused on accurately capturing the prominent noise sources at both flap tips for the baseline configuration. Then, we evaluated the effectiveness of a novel noise reduction concept applied to the flap tips. The time-accurate simulations were obtained using the NASA Langley FUN3D unstructured Navier-Stokes flow solver and the Exa Corporation PowerFLOW Lattice-Boltzmann flow solver. Approximately one billion volumetric cells were used to discretize the space surrounding the aircraft surfaces.

Results and Impact

Our simulations have provided unique and detailed insight into the prominent fluid dynamical processes that create noise at the flap tips. Scrutiny of the flow field in the vicinity of the tips revealed the formation/presence of multiple vortices that behave like miniature tornados. Their evolution, merging, and interaction with the sharp corners at the tips produce high-amplitude sound waves that propagate towards the ground. We also demonstrated that the noise abatement concept applied to the tips is very effective.

Role of High-End Computing Resources and Services

The vast number of arithmetic operations needed to perform any of our simulations requires usage of the largest supercomputers. All the simulations were performed on NASA's Pleiades supercomputer using approximately two thousand processors. Depending on the nature of the needed information, the computational runs could last from two weeks to two months, resulting in several Petabytes of data. The rendering and effective visualization of such massive datasets were made possible by the members of the NAS visualization group at NASA Ames.

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Demo 5

Modeling of Extended Formation Flight on High-Performance Computers

Overview

As in avian flight, aircraft flown in formation can obtain significant savings in induced drag due to favorable upwash of the lead aircraft. As the world's fleet of aircraft grows, formation flight is one approach toward reducing fuel consumption on long-range flights. NASA's Fundamental Aeronautics project is studying this concept as one wedge in a comprehensive strategy toward reduced carbon emissions and fuel consumption. While formation flight has been studied since the early 1900's, estimates of the potential benefits have varied significantly. Credible estimates of induced drag savings of 10-30% have been predicted by low-order methods but have been difficult to confirm with high-fidelity simulations.

Project Details

Even with modern computing hardware, these simulations pose a significant challenge since they hinge on accurately predicting and measuring induced drag of complete aircraft at transonic conditions and accurately propagating vortices and wakes over long distances through a computational domain. In extended formation flight, operational safety dictates separation distances of 15-50 spans, further increasing the level of difficulty.

These challenges are met by using a non-body-fitted simulation approach on meshes which dynamically adapt to minimize errors in the measurement of induced drag of the aircraft in formation. The simulations include the effects of flow compressibility, aircraft trim, control surface deflection and other important physics which are lacking in previous work.

Results and Impact

Results from these simulations are verified with flight-test data being run cooperatively with other government agencies. After validation, these data are used in models of the National Airspace System to quantify the potential of formation flight to reduce fuel consumption at a national scale.

Role of High-End Computing Resources

Formation flight involves aerodynamic phenomena spanning lengths from millimeters to miles. This extraordinary range of scales and the sensitivity of the output to error in the simulation make these extremely challenging problems. With problem sizes that are on the order of a billion degrees of freedom, and hundreds of cases to consider, the availability of NASA's high-end computing resources are the key to this research.

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HUMAN EXPLORATION OPERATIONS (HEOMD)

Demo 6

Supersonic Retropropulsion for Mars Entry

Overview

Supersonic Retropropulsion (SRP) is a potential method of decelerating high mass vehicles entering the Martian atmosphere. This technology, which employs jets opposing a supersonic freestream, is needed because current methods of supersonic deceleration do not scale to human exploration or large robotic sized spacecraft. Computational Fluid Dynamics (CFD) is important to the development of SRP because flight and ground testing is difficult and cost-prohibitive at these flow conditions. To validate CFD at these conditions, three NASA flow solvers were employed and two wind tunnel tests were conducted allowing code-to-code and code-to-test comparisons. The comparisons are positive and show that CFD is capable of simulating SRP.

Project Details

Three NASA-developed Navier-Stokes flow solvers were used in a CFD validation effort for SRP. The codes are Data Parallel Line Relaxation (DPLR), Fully Unstructured Navier-Stokes Three-Dimensional (FUN3D), and OVERset grid FLOW solver (OVERFLOW). Two wind tunnel tests were completed with the specific purpose of CFD validation. The tests were conducted in the Langley and Ames Unitary Plan Wind Tunnels, and produced surface pressure data as well as high speed flow visualization imagery. Qualitative and quantitative comparisons between codes and test data show a high capability of CFD to simulate SRP flowfields.

Results and Impact

The capability of CFD to simulate SRP flowfields will allow CFD to be used for parametric studies, vehicle control and stability analysis, and properly predicting the complex physics of SRP at Martian entry conditions.

Role of High-End Computing Resources and Services

The CFD validation studies required time-accurate simulations, which used millions of processor hours and created terabytes of data. NASA supercomputing resources not only made an analysis of this size possible, but also enabled the project to complete the computations efficiently in a timely manner.

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Demo 7

Validating Water Spray Simulation Models for the SLS Launch Environment

Overview

NASA regularly uses computational fluid dynamics (CFD) simulations to assess the loads and risks for space vehicles at liftoff. Traditionally, these simulations have been used to make predictions either near the vehicle, such as for plume recirculation, or for large scale effects like wind. However, validations against recent test data have shown that modern codes have the capability to make meaningful pressure predictions over the full launchpad for frequencies up to 150 Hz. This limit is high enough that significant phenomena, like the transient startup and overpressure pulse of rockets, can be modeled.

While the results of these validations have allowed CFD to make immediate impacts on the design of NASA's new Space Launch System, they have also been primarily for dry launchpads. To examine the full range of designs, CFD also needs to incorporate multi-phase components like water sprays. To enable this work, such a capability was developed in partnership with Mississippi State, and then used to simulate the effects of water suppression for a second validation case.

Project Details

For this project, the emission, flight, and evaporation of water spray systems on an active launchpad was simulated using a two-phase approach of lagrangian water particles and gas phase CFD elements. The simulation was based on a test case from the Ares Scale Model Acoustic Test so that pressure predictions from across the launchpad could be validated against real data. Approximately 200 million cells of resolution were used to capture the fine detail and geometry of the pad, and millions of particles were tracked to capture the dynamics of a water cascade. This work was performed using a density-based finite-volume CFD program called Loci/CHEM.

Results and Impact

Ignition overpressure and payload acoustics are design considerations which are consistently risk drivers for new launch vehicles. Traditionally, these effects have been predicted using analytical methods, with low-fidelity scaling of results from old designs. However, the technology development and validation efforts supported by this work are allowing CFD to make validated predictions of pressure over a full launchpad using the geometry as designed for a specific vehicle. Rather than relying solely on "rules of thumb" to guide suppression strategies, such systems can be optimized for maximum effect using

CFD parametrics Furthermore, problems with these systems can be identified and fixed before metal is ever cut, providing significant cost savings to NASA.

Role of High-End Computing Resources and Services

Prediction of acoustic effects with CFD for a structure the size of a launch pad is an intense computational task, and one which would be extremely difficult without the resources of a supercomputer like Pleiades to support it. Simulations of even a scaled rocket took nearly a week to complete while running on over 1000 processors, and were normally executed in groups of two or more to test design permutations. In addition, the storage requirements for such simulations were on the order of terabytes per simulation, with regular processing of hundreds of individual gigabyte scale files necessary for visualization, post-processing, and analysis of data.

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Demo 8

Simulating Moving Valves for Space Launch System Liquid Engines

Overview

Three-dimensional, time accurate fluid dynamics analysis of moving valves offers tremendous insight for valve design and operation. Fluid dynamics that occur during valve actuation often have significant impact on the valve and connected hardware. However, due to a lack of computational resources, fluid dynamic analysis of transient valve motion is rarely performed as part of a valve design process.

In some valve applications, such as the Space Shuttle Orbiter Flow Control Valve (FCV), the first sign of significant fluid dynamics caused by valve actuation was the fluid induced high cycle fatigue failure of the valve poppet. Computational Fluid Dynamics analysis performed at Marshall Space Flight Center using the density-based fluid analysis program LOCI\Chem succeeded in identifying fluid mode shapes and amplitudes that could have possibly caused the FCV to fail. The analysis indicated that the exact conditions that led to the valve failure probably occurred at some point during the valve actuation. However, due to limitations of the CFD tools and processing power available in 2009, all analysis was performed with the valve in a fixed, static position. The inconclusive results of the static position FCV analysis and the associated delays in the Orbiter flight schedule caused by the valve failure emphasized the real need to develop the ability to perform time-accurate computational fluid dynamics analysis of moving valves.

Marshall Space Flight Center has developed the ability to model large-scale moving valve simulations using LOCI\Chem. Due to the efficient parallelization of LOCI\Chem and the increased computational resources available at NASA's Ames Research Facility, moving valve simulations are completed quickly enough to support valve design cycles.

Project Details

For this project, the opening and closing cycle of a candidate Space Launch System FCV is modeled to evaluate potentially damaging unsteady fluid environments in the valve and other critical performance metrics. Simulations were conducted using LOCI\Chem with an

overset mesh method to simulate the moving valve components. A hybrid unstructured mesh with ~55 million cells was required to resolve the fluid dynamics of interest. A hybrid Reynolds-Averaged Navier-Stokes/ Large Eddy Simulation (hybrid RANS-LES) turbulence model was used to accurately capture time-accurate pressure oscillations in the flow.

Results and Impact

CFD analysis of the moving valve identified the onset of a periodic pressure response in the flow which only occurs after the valve re-opens from closure. The analysis showed that the tool holes downstream of the flow orifices were contributing to a 14Khz pressure oscillation in the flow. A recommendation to fill the tool hole with an insert was given to the valve vendor. The vendor recognized the benefit of eliminating this source of unsteady fluid environments and incorporated the recommendation into the design. The analysis also quantified the unsteady forces on the poppet head due to pressure changes during actuation.

Role of High-End Computing Resources and Services

In order for the CFD analysis to provide input for the valve design cycle simulations were massively parallelized on NASA's Pleiades supercomputer. Simulations were performed using approximately 600 processors in order to complete one closing and re-opening cycle in a working week.

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Demo 9

Innovative Simulations for Modeling the SLS Solid Rocket Booster Ignition

Overview

NASA's new heavy launch vehicle, known as the Space Launch System (SLS), will utilize 2 five-segment reusable solid rocket motors (RSRMV), as boosters. The results of RSRMV static test firings to date suggest an interaction between the booster and the thrust stand dynamics is likely compromising test data, especially the critical thrust rise rate, during motor ignition. Also there is a need accurately characterize the RSRMV ignition transient to provide high-fidelity inputs for SLS launch-induced environments simulations. Multiple time accurate, 3D computational fluid dynamics (CFD) simulations have been performed using the Loci-Chem code on NASA's supercomputing resources to model the first half-second of the RSRMV ignition transient to address both of these issues.

Project Details

Time-accurate, fully 3-D CFD simulations of the RSRMV ignition transient were performed using the Loci-Chem code. A transient, pressure vs. time boundary condition was applied to the motor igniter. The simulations incorporated an updated Loci-Chem ignition module that solves the 1-D heat equation into the propellant grain to determine when each individual propellant surface cell should ignite. When ignited, the propellant "burns" using an empirical boundary condition based on propellant formulation and local pressure. The combustion products were modeled as a homogenous, single species gas.

Validation efforts have included an input sensitivity study in which different boundary conditions were applied based on parametric values for inputs such as burn-rate and gas properties. Grid and time step parametrics have been done for solution verification. The grid sensitivity study used meshes ranging from 90-250 million total cells. The time-step study used time-steps ranging from 1-5 microseconds.

Results and Impact

CFD head end pressure results and thrust calculations match very well with static test data. Animations were created to facilitate identification of the fluid mechanisms that affect the motor pressure rise rate. Since the CFD simulations do not factor in thrust stand dynamics, the simulations are being used to identify thrust stand dynamics contributions to the measured thrust.

Over 100 numerical probes were placed in a plane located at the entrance of the nozzle to capture the fluid properties of the gas at regular time-intervals. These were used to create a 3-D fluid dynamics profile for an input boundary condition for additional CFD simulations for SLS launch-induced environments.

Role of High-End Computing Resources and Services

Utilizing NASA's Pleiades supercomputer cluster, has allowed execution of multiple cases simultaneously. The performance of Loci-Chem scales very efficiently as the number of processors is increased. Using 2,400 processors per simulations allows completion in 2 weeks. This turnaround time enables support of RSRMV and SLS during the design and development phases. NASA's LOU archival system has also been necessary to store the several terabytes of data produced by each simulation.

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Demo 10

Solid Rocket Booster Ignition Overpressure Simulations for the Space Launch System

Overview

During launch, the Space Launch System (SLS) vehicle now in development will experience a series of large pressure waves emanating from the flame trench below which are caused by the fast ignition transient of the solid rocket boosters (SRBs), and have the ability to cause damage to the vehicle. While this ignition overpressure (IOP) phenomenon was observed during the Space Shuttle program, the existing engineering-level IOP analysis tools could not account for the different configuration of the SLS vehicle and launch pad. To study the effects of these differences, we performed time-accurate computational fluid dynamics (CFD) simulations of the SLS IOP event using NASA's supercomputing resources.

Project Details

The goal of this work was to resolve multiple uncertainties which existed in the IOP analysis, including: the interaction of the SRB IOP with the core stage liquid engines at full

power, effects of the new SLS mobile launcher design, and possible design changes to the flame deflectors below the vehicle.

Several simulations were performed with varying levels of fidelity in order to specifically address each of these uncertainties and include updated vehicle and mobile launcher designs. Between 50 million and 150 million computational cells were used to model the detailed structures of the SRB and core stage plumes within the complex launch pad geometry. The simulations were realized with a CFD code named Loci/CHEM, using thousands of processors in parallel.

Results and Impact

Of the various uncertainties addressed in this work, the analysis of our simulations showed that the interaction of the SRB and core stage plumes had the most significant impact on the IOP environment. Because the core stage engines are at full power at the time of SRB ignition, the IOP wave is partially entrained or dissipated by the core stage plume flow field which creates smaller, less coherent waves with lower amplitude. In turn, the IOP wave interaction with the vehicle was more localized and peak impingement pressures were reduced.

These and other findings were used to improve the IOP analysis which is provided to the SLS vehicle designers by removing unnecessary levels of conservatism. In addition, the higher fidelity simulations were used to modify parameters in the IOP analysis tools such that the predicted IOP waveform was reflective of the SLS vehicle and mobile launcher configuration, rather than being anchored to early Space Shuttle data.

Role of High-End Computing Resources and Services

Due to the time-sensitive nature of producing the IOP analysis for the SLS vehicle design cycles, the use of NASA's supercomputing resources was vital to completing this work. Each simulation was run with thousands of processors on the Pleiades cluster, required 7 to 15 days to complete, and produced over 2 terabytes of data.

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Demo 11

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Demo 12 Modeling and Simulation Support for NASA's Next-Generation Space Launch System

Overview

Computational Fluid Dynamics (CFD) simulations are being performed to support the design of NASA's next generation launch vehicle, the Space Launch System (SLS). Modeling and simulation support includes characterizing the aerodynamic performance of the vehicle for a suitable ascent trajectory, determining the distributed aerodynamic line loads along the vehicle for structural analysis, and providing surface pressure signatures to assist in venting design for components of the vehicle.

Project Details

During the early design of the SLS, focus is placed on the stability and control of the vehicle during ascent and maintaining structural integrity throughout the mission. Characterization of the aerodynamic environments plays a key role in providing the necessary inputs for the Guidance Navigation and Control and the Structural Loads groups. In order to determine these environments before the vehicle is built, CFD simulations of SLS are performed at select points over the ascent trajectory and multiple angles of attack. The integrated and distributed aerodynamic loads on the vehicle are then extracted from the CFD solution and provided as input data for trajectory and structural analysis which are used to improve the design of the vehicle.

In addition to providing information to modify the exterior shape and the interior structural components of the SLS, surface pressures over specific components of the vehicle are extracted and provided to the Venting group. This data is then used to determine where proper venting should occur along the vehicle.

Results and Impact

CFD simulations have been used to aid in critical design decisions for SLS early in the design cycle when wind tunnel data was not yet available. The

CFD Simulations to Support the Next Generation Pads

Overview

With the retirement of the Space Shuttle, NASA's new heavy-lift capability, the Space Launch System, in addition, commercial vehicles such as SpaceX's Liberty and ULA's Delta IV Heavy and Atlas V are being considered for transporting crew/cargo to the International Space Station (ISS). To accommodate these vehicles, Kennedy Space Center (KSC) is evaluating their launch site capabilities. Components of the pad are the Flame Trench and the Main Flame Deflector whose main purpose is to safely deflect the exhaust away from the vehicle as it lifts off.

Project Details

Re-design of the Main Flame Deflector (MFD) and assessment of its performance regarding containment plume in the trench, pressure and thermal loads and the surrounding environment for the launch of commercial vehicles. A Computational Fluid Dynamics approach is well suited to provide the necessary capabilities during a rapid design cycle. Through examination of the concern areas, incremental studies and comparative studies of various MFD designs can be achieved in a time and cost efficient manner. This project consists of a CFD effort undertaken by the Applications and Simulation branch at NASA Ames Research Center in support of the MFD re-design project.

Results and Impact

This project assesses candidate MFD designs and provides vehicle configurations and layouts and provides data during the design cycle. Specifically, analysis includes containment characteristics, time evolution of temperature and heat transfer rate distribution over trench surfaces.

Role of High-End Computing Resources and Services
Each of these simulations require roughly a week of time using up to 960 Westmere cores on NASA's supercomputer. Since the simulations are unsteady, terabytes of data is generated for each calculation and analysis and visualization is conducted using high performance systems, including in-house part and other software.

Researcher: Michael Barad, NASA Ames Research Center

ongoing modeling and support effort is making a large impact on import design decisions including:

- Down selecting from several vehicle shapes
- Outer Mold Line (OML) of the vehicle
- Structural analysis of the core-stage and protuberances
- Core-stage main engine hinge moment analysis

CFD support for SLS will continue to advance as the vehicle matures and will make major impacts on:

- Booster separation analysis
- Core-stage fairing and main engine layout
-

Role of High-End Computing Resources and Services

NASA's Advance Supercomputing facilities enable fast and efficient turnaround time for CFD simulation support of SLS. The Pleiades machine allows viscous databases including several hundreds of simulations to be completed in under a week using 300 cores and 40 hours of wallclock time per simulation.

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SCIENCE MISSION DIRECTORATE (SMD)

Demo 13

Simulating Planetary Entry Environments for Space Exploration Vehicles

Overview

One of the challenges in designing a spacecraft for planetary entry is to predict the heating on the surface of a vehicle. It is important that designers have an accurate estimate of the aerothermal environment so they can select appropriate Thermal Protection System (TPS) materials and determine the TPS thickness required to protect a spacecraft from its high-speed entry into a planet's atmosphere. Since it is impossible to reproduce the exact flight conditions with ground-based experiments, we must rely on computer simulations to predict worst-case thermal environments and to extrapolate test data to flight-like conditions.

Project Details

For the Mars Science Laboratory (MSL) and the Orion Multi-Purpose Crew Vehicle (MPCV) projects, Computational Fluid Dynamics codes were used to estimate the aerothermal environments at flight and at ground-based test conditions. These simulations, along with experimental data, were used to verify the accuracy of our computer models, to establish uncertainties of the heating estimates, and to study differences of various turbulence models.

Results and Impact

Our research revealed that even on a smooth body, it is difficult to accurately predict the heating on the separated backshell; therefore, large safety margins are needed when designing the backshell TPS. Simulations using a more complex two-equation Shear Stress Transport turbulence model did not perform better than the algebraic Baldwin-Lomax or the one-equation Cebeci-Smith turbulence model.

Role of High-End Computing Resources and Services

Since a typical simulation required more than 70 hours using 1,000 Pleiades cores, it is unfeasible to run hundreds of these calculations without the high-end computing resources at NAS. NASA's Pleiades supercomputer played a critical role in the generation of aerothermal databases for the MSL and Orion MPCV programs.

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Demo 14

NASA Center for Climate Simulation Highlights

Overview

The NASA Center for Climate Simulation (NCCS) offers integrated supercomputing, visualization, and data interaction technologies to enhance NASA's weather and climate prediction capabilities. It serves hundreds of users at NASA Goddard Space Flight Center as well as other NASA centers, laboratories, and universities across the U.S.

Project Details

Over the past year, NCCS has continued expanding its data-centric computing environment to meet the increasingly data-intensive challenges of climate science. We doubled our Discover supercomputer's peak performance to more than 800 teraflops by adding 7,680 Intel Xeon Sandy Bridge processor-cores and, most recently, 240 Intel Xeon Phi Many Integrated Core (MIC) co-processors.

A supercomputing-class analysis system named Dali gives users rapid access to their data on Discover and to high-performance software, including the Ultrascale Visualization Climate Data Analysis Tools (UV-CDAT). Analysis and visualization interfaces range from user desktops to a 17- by 6-foot hyperwall. NCCS is also exploring highly efficient climate data services and management with a new Hadoop Map/Reduce cluster while augmenting its data distribution to the science community.

Results and Impact

Using NCCS resources, NASA completed its modeling contributions to the Intergovernmental Panel on Climate Change (IPCC) Fifth Assessment Report this summer as part of the ongoing Coupled Model Intercomparison Project Phase 5 (CMIP5). Ensembles of simulations run on Discover reached back to the year 1000 to test model accuracy and projected climate change through the year 2300 based on four different scenarios of greenhouse gases, aerosols, and land use.

The data resulting from several thousand IPCC/CMIP5 simulations—as well as a variety of other simulation, reanalysis, and observation datasets—are available to scientists and decision makers through an enhanced NCCS Earth System Grid Federation Gateway. Worldwide downloads have totaled over 110 terabytes of data.

Additional science highlights include a 10-kilometer-resolution simulation of global aerosols, modeling support for flight-based field campaigns by NASA and collaborating agencies, and study of the factors leading to spring 2011 extreme weather events including floods and tornadoes.

Role of High-End Computing Resources and Services

For their IPCC simulations, NASA's Goddard Institute for Space Studies and Global Modeling and Assimilation Office used up to 160 concurrent jobs and 18,000 cores on Discover to simulate the breadth of CMIP5 scenarios. In aggregate, they completed tens of thousands of simulation-years and consumed more than 300 million Intel Xeon core-hours.

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Demo 15

Ultrascale Climate Data Visualization and Analysis

Overview

Earth system scientists are being inundated by an explosion of data generated by ever-increasing resolution in both global models and remote sensors. Advanced tools for accessing, analyzing, and visualizing ultra-scale climate data are required to maintain rapid progress in Earth system research. To meet this need, the NASA Center for Climate Simulation (NCCS) at Goddard Space Flight Center is developing an advanced computational infrastructure that can provide high-performance analysis and visualization capabilities to the desktops of climate scientists.

Project Details

In collaboration with the Ultra-scale Visualization Climate Data Analysis Tools (UV-CDAT) development consortium, NCCS is developing climate data analysis and visualization tools for UV-CDAT, which provides data analysis capabilities for the Earth System Grid (ESG). These tools feature workflow interfaces, interactive 3D data exploration, hyperwall and stereo visualization, automated provenance generation, and parallel data processing. NASA's DV3D is a UV-CDAT package that enables exploratory analysis of diverse and rich data sets stored in the Earth System Grid Federation (ESGF). DV3D provides user-friendly workflow interfaces for advanced visualization and analysis of climate data at a level appropriate for scientists.

Results and Impact

These computational services allow unprecedented access to high-performance data processing applications in support of Earth system science, facilitating climate data

analysis operations that would otherwise be very difficult or impossible. This effort directly supports NASA's mission to use remote sensing data and global models to better understand the dynamics of the Earth system. Analysis of observational and model data is essential in understanding how changes to Earth system processes, such as the climate, will impact humankind.

Role of High-End Computing Resources and Services

DV3D's seamless integration with CDAT's climate data management system (CDMS) and other climate data analysis tools provides a wide range of climate data analysis operations, e.g. simple arithmetic operations, regridding, conditioned comparisons, weighted averages, various statistical operations, etc. Several teams are developing parallel versions of these tools that will enable users to analyze and display large data sets that cannot currently be processed with existing desktop tools. This enables scientists to run analyses that were previously intractable due to the large size of the datasets and, using DV3D, seamlessly couple these analyses with advanced visualization methods.

Researcher and Presenter at SC12:

Thomas Maxwell, NASA NCCS

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Demo 16

NASA Climate Simulations and Observations for the IPCC and Beyond

Overview

Exploiting more than 30 years of global satellite observations, NASA scientists are creating observation-driven climate simulations that improve our insights into both climate model behavior and the complex physical processes and feedbacks that influence the Earth's climate.

NASA's near- and long-term climate simulations and observations are contributing to international efforts such as the Coupled Model Intercomparison Project Phase 5 (CMIP5) and the Fifth Assessment Report of the International Panel on Climate Change (IPCC AR5), in addition to the US's monthly National Multi-Model Ensemble (NMME) and the next quadrennial National Climate Assessment (NCA) in 2013.

Project Details

NASA's global climate simulations and satellite observations allow us to explore evolution and variability of the Earth system from a variety of perspectives and time scales.

- Researchers at the Goddard Institute for Space Studies (GISS) focus on long-term climate simulations from decades through centuries using their ModelE General Circulation Model (GCM) coupled with the Russell or HYCOM ocean model.
- For nearer-term seasonal to decadal climate time scales, the Global Modeling and Assimilation Office (GMAO) applies its GEOS-5 Atmosphere-Ocean GCM.
- To advance use of climate simulation results and related satellite observations and analyses, NASA serves the data via Earth System Grid Federation (ESGF) nodes on <http://esgf.nccs.nasa.gov/> and <http://esgf-datanode.jpl.nasa.gov/>.

GISS's Panoply tool (<http://www.giss.nasa.gov/tools/panoply/>) allows researchers to quickly visualize NASA's climate simulation data, while NASA's collaborations with the UV-CDAT project (<http://uvcdat.llnl.gov/>) support analysis capabilities such as interactive 3-D data exploration.

Results and Impact

NASA's historical climate hind-casts and observation-driven near- and long-term simulations contribute to scientists' understanding of the complicated interactions of climate's physical processes. NASA's collections of satellite observations since 1979 provide scientists with essential data for analysis and comparison with model results. Taken together, the analysis of these near- and long-term climate observations and simulations significantly improves our understanding of Earth's climate and climate models, and the resulting range of future climate change estimates are of great value for IPCC AR5 investigators, other scientists, and policymakers considering possible consequences.

Role of High-End Computing Resources and Services

GISS and GMAO climate simulations run on the Discover supercomputer at the NASA Center for Climate Simulation. From June 2010 through July 2012, climate processing has consumed more than 300 million core-hours and produced more than 60,000 simulation-years.

Researcher and Presenter at SC12:

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Demo 17

Next-Generation Climate Data Services: MERRA Analytics

Overview

Scientific data services are critical to the mission of the NASA Center for Climate Simulation (NCCS). Modern Era Retrospective-Analysis for Research and Applications/Analytic Services (MERRA/AS) is a cyber infrastructure resource for developing and evaluating the next generation of climate data analysis capabilities. MERRA/AS supports Obs4MIPs (observations for model inter-comparison projects) activities by reducing the time spent in the preparation of MERRA data used in data-model inter-comparison. It also provides a testbed for experimental development of high-performance analytics.

Project Details

MERRA/AS is a cloud-based service built around the Virtual Climate Data Server (vCDS) technology that NCCS currently uses to deliver Intergovernmental Panel on Climate Change (IPCC) data to the Earth System Grid Federation (ESGF). Crucial to their effectiveness, MERRA/AS's servers use a workflow-generated realizable object capability to perform analyses over the MERRA data using the Hadoop/MapReduce approach to parallel storage-based computation.

Results and Impact

The results produced by these operations will be stored by the vCDS, which will also be able to host code sets for those who wish to explore the use of Hadoop/MapReduce for more advanced analytics. While the work described here will focus on the MERRA collection, these technologies can be used to publish other reanalysis, observational, and ancillary Obs4MIPs data to ESGF and, importantly, offer an architectural approach to climate data services that can be generalized to applications and customers beyond the traditional climate research community.

Role of High-End Computing Resources

Powerful computing resources are necessary for on-demand analytic processing across 30+ years of MERRA reanalysis data. The MapReduce operations leverage a cluster consisting of 36 Dell R710 servers each populated with twelve (12) 3-terabyte hard drives in addition to their operating system disks (CentOS 6.3). For interconnectivity, there is a 36-port Fourteen Data Rate (FDR) InfiniBand (IB) switch plus a 48-port Gigabit Ethernet switch. Initial cluster metrics show one-way IB performance rates topping 6,000 megabytes per second, peaks of 314 gigaflops per server, and an overall capability of approximately 11 teraflops.

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Presenter at SC12:

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Demo 18

Recent Advances in High-Resolution Global Atmospheric Modeling

Overview

High-resolution global atmospheric modeling provides a unique tool to study the role of weather within the global climate system. The Goddard Earth Observing System Model, Version 5 (GEOS-5) is capable of simulating global weather at resolutions of 10 to 3.5 kilometers (km) globally. These Global Earth-system Mesoscale Modeling (GEMM) simulations with GEOS-5 represent multiple scales of atmospheric phenomena—from convective clusters of deep convection, to hurricanes, to large mid-latitude storm systems—within a unified simulation of the global circulation.

Project Details

GEMMs with GEOS-5 produce a realistic representation of our atmosphere at resolutions comparable to many satellite observations. This provides an opportunity to perform comprehensive process studies on the formation of regional weather events and their impact on seasonal climate, improve the integration of existing observations into our data assimilation systems, and explore the potential of new observations through observing system simulation experiments.

GEOS-5 uses the Goddard Chemistry Aerosol Radiation and Transport (GOCART) model within these GEMM simulations to include the global transport and direct radiative impacts of aerosols. These aerosols include dust particles lifted from the Earth's surface by strong

winds and deep convection, sea-salt blown from the ocean surface, plumes of sulfates from volcanic eruptions and fossil fuel emissions, and organic and black carbon within smoke from wildfires and human-initiated burning. These tiny particles can be transported large distances from their sources as they get caught up in the strong winds of the atmospheric circulation and have a significant impact on air quality, visibility, and human health.

Results and Impact

A 2-year GEMM simulation at 10-km resolution with GEOS-5 provides our first look at the potential of high-resolution global simulations integrating global weather phenomena within the variability of seasonal climate change. The 10-km GEMM simulation captured the dynamic variability of North Atlantic tropical cyclone activity for the very active 2005 season and the more typical 2006 season. While resolution does improve the simulated variability of tropical cyclone formation, it is also a key element in improving the intensity of tropical cyclones that form within the model. At 10-km resolution the GEOS-5 GEMM simulations begin to represent the strongest hurricanes with near surface winds in excess of 160 miles per hour.

Role of High-End Computing Resources and Services

The 2-year, 10-km GEOS-5 GEMM simulation ran on 3,750 processors of the Discover supercomputer at the NASA Center for Climate Simulation for several weeks and produced over 400 terabytes of data. Experimental versions of GEOS-5 at 3.5-km global resolution represent the future of global atmospheric modeling including non-hydrostatic dynamics, cloud microphysics, and interactive aerosols (known within the community as global cloud-resolving models). This class of global models requires more than 20 times the computational capability of the Discover supercomputer to complete a 5-day forecast within the operational requirements of our data assimilation system.

Researcher and Presenter at SC12:

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Demo 19

Causes and Consequences of Turbulence in the Earth's Protective Shield

Earth and other planets are engulfed in the Sun's atmosphere, which extends to about 10 billion miles! The Earth's dipole magnetic field shields us from most of the Sun's effects and its frequent storms. However, the shielding is not perfect, and the solar wind is able to penetrate ("crack") the magnetosphere.

Our petascale kinetic simulations are critical to the development of a more complete understanding of the cause and conditions for the development of this crack in the magnetosphere, which can affect the Earth and its technological systems, and has caused over \$4 billion in satellite losses alone. In this project we have:

Used simulations with over 3 trillion particles to study the causes and consequences of turbulence in the magnetosphere

Discovered mechanisms for the generation of the turbulence.

Used 3D global simulations to examine the global consequences of the turbulence.

Achieved closure on a number of longstanding issues on this topic, such as the role of certain type of waves in reconnection

Confirmed several of our predictions through comparison with spacecraft observations

Petascale simulations on massively parallel systems such as NASA's Pleiades supercomputer have been crucial to our breakthrough studies and are enabling closure on critical issues in magnetospheric physics.

Researchers:

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Presenter at SC12:

Ari Le; University of California, San Diego/SciberQuest, Inc.

Demo 20

NASA Earth Exchange (NEX): A Collaborative Supercomputing Platform

Overview

The NASA Earth Exchange (NEX) represents a new collaboration platform for the Earth science community that provides a mechanism for scientific collaboration and knowledge sharing. NEX combines state-of-the-art supercomputing, Earth system modeling, workflow management, and NASA remote sensing data feeds to deliver a complete work environment in which users can explore and analyze large datasets, run modeling codes, collaborate on new or existing projects, and quickly share results among the Earth science communities.

Project Details

The main goal of NEX is to enable enhanced and more efficient use of Earth observations for NASA Earth science technology, research and applications programs.

NEX utilizes the Pleiades supercomputing platform together with over 1PB of satellite, climate and model datasets in order to accelerate research in the Earth sciences. The results and project details can then be shared with the community through the NEX portal – a web-based knowledge network. Finally, NEX capabilities include a state-of-the-art collaboration facility that enables distributed teams to work together and share with the rest of the community through seminars and other outreach activities.

Results and Impact

As the development of NEX continues, it strives to lower the barrier of entry to data- and computer-intensive science. NEX will provide a mechanism for continuous engagement among members of the global science communities to work together to address grand challenge problems in Earth sciences.

Role of High-End Computing Resources and Services

The Pleiades supercomputing architecture combined with the massive data store and high-speed network enables NEX to engage large scientific communities and provide them with capabilities to execute modeling and data analysis on a grand scale, which was not previously achievable by most scientists. In one of the recent application of NEX, a team of researchers from NASA and South Dakota State University used the system to derive a new global vegetation product from over 80,000 Landsat scenes in order to provide a dynamic view of changing vegetation over the course of the year at 30-meter resolution. The processing of nearly 5 trillion pixels took only few hours on NEX, providing an unprecedented monitoring capability at a global scale.

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Demo 21

Powering Deep Space Missions: Thermoelectric Properties of Complex Materials

Overview

Thermoelectric materials are used to generate electric power from the decay of radioisotopes in deep space mission spacecrafts. Over the past decades only very simple materials (such as silicon and bismuth telluride) have been used for space application but experimentalists at JPL are studying more complex materials (such as La₃Te₄, zintl, and skuterrudites) with better efficiency. The objective of this project is to use state-of-the-art electronic structure calculations to compute thermoelectric properties of complex materials and guide the synthesis in the laboratory of materials with improved thermoelectric properties.

Project Details

The figure of merit for thermoelectric materials is proportional to the square of the Seebeck coefficient, which measures the electric field that arises in a material in response

to an applied temperature gradient. This work focuses on computing the Seebeck coefficient for complex materials using first principles electronic structure calculations. The first principles electronic structure is obtained from the density functional theory, where the many body interaction between the electrons is approximated by a one-electron potential. The electronic structure is used to compute the Seebeck coefficient from a solution of the Boltzmann transport equation.

We use the community software package Quantum Espresso (www.quantum-espresso.org) to compute the electronic structure. The computationally most costly numerical algorithms in Quantum Espresso are FFTs and orthogonalizations of large vector sets.

Results and Impact

We calculated the band structure, electronic density of states and Seebeck coefficient for La₃Te₄ and several zintl materials. We validated our modeling approach by comparing our results with published calculations and with measured data when available. We found excellent agreement.

We found that the substitutions of appropriately chosen elements at the atomic level can alter the Seebeck coefficient. These exploratory studies have prompted new experiments that are expected to lead to the discovery of materials with improved figure of merit, as predicted by our calculations.

Role of High-End Computing Resources and Services

A typical first principles electronic structure calculation for complex materials takes up to 6 weeks of computing time up to 200 processors. The memory requirements are about 439 MB per process and 589 GB of disk space. These calculations cannot be performed on desktop computers, and supercomputing resources are essential.

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Demo 22

Meeting NASA's High-End Computing Goals Through Innovation

Overview

Located at the NASA Advanced Supercomputing facility between San Francisco and San Jose, California, the High End Computing Capability (HECC) Project provides NASA scientists and engineers with a world-class computing environment to facilitate advances in their areas across all NASA technical mission directorates. The HECC project's computing environment and full range of supporting services is focused on enabling discovery across a wide array of disciplines. Over the past year, HECC expanded Pleiades to over 1.7 PF, tripled the archive storage capability to over 90 PB, expanded the available tool set for diagnosing application performance and improved the ability of the security software to detect and prevent hostile actions taken against the computer environment.

Project Details

Since its inception in 2004, HECC has maintained a computing environment balanced by a strong set of related services. This combination of hardware supported by the services

enables exciting innovations in science and engineering. The HECC hardware expanded in 2012 reaching a theoretical peak processing capability exceeding 1.7 PF on Pleiades and tripled the archive capability to over 90 petabytes. Maintaining the capability of large shared-memory application development with single-system images of up to 4 terabytes and providing an internationally acclaimed data analysis and visualization capability providing both concurrent and traditional visualization capabilities joins with the additions to provide a unique discovery environment.

The services attached to the facility provide a robust discovery environment focused on the success of our user community. This past year has seen improvements across the board with a strong focus on more useful tools, a strong outreach through a series of technical webinars, and a website designed to address our users challenging needs.

Results and Impact

HECC has been successful in providing a cost-effective, productive compute environment. The facility has been able to support a wide variety of users with a broad range of job requirements. The successes have ranged from supporting current flying missions such as Kepler and UAVSAR to research into the formations of the universe.

Many of the key successes enabled through the HECC program are being highlighted in other areas of our booth at SC12. The successes highlighted by this project are the installation and integration of the new Sandy Bridge nodes adding FDR into the InfiniBand fabric, increasing the hypercube to a twelfth dimension and the growth of the archive.

Role of High-End Computing Resources and Services

The HECC project's role is to provide all of NASA with a cost-effective, reliable, state-of-the-art supercomputing capability. Through strong relationships with the vendor community and a strong technical team, HECC continued its achievement of this role in 2012.

Researcher and Presenter at SC12:

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Demo 23

Continuous Enhancements to the Pleiades Supercomputer for Maximum Uptime

Overview

When Pleiades was initially installed in 2008, the system was a homogeneous cluster with 51 thousand cores and Double Data Rate InfiniBand. Since then, the system has been increased by nearly 2.5x to 126 thousand cores with 4 different generations of processors and 3 generations of (DDR, QDR, and FDR) InfiniBand in a single cluster. This has challenged the HECC systems team to develop tools and processes to maintain a productive operational supercomputer with minimal downtime.

Project Details

Operating an InfiniBand cluster of nearly 12,000 nodes requires the HECC systems team to be able ensure that the InfiniBand interconnect for the system is robust to handle fault conditions and to be able to recover gracefully. One of the enhancements developed was a modification to the InfiniBand Subnet Manager to enable the live integration or removal of

nodes from the InfiniBand fabric. This ability allowed the system to continue to provide computing cycles at the same time that resources added to the system or removed for maintenance activities.

Another enhancement to the system was feature of suspend and resume of the batch scheduler software. By stopping jobs on the system, this enabled some maintenance activities without needing to drain the system for maintenance time, which is an expensive process in terms of lost computing cycles. By suspending jobs on the system, the overhead maintenance time can be greatly reduced with minor impact on the users.

A related improvement to the batch scheduler is the ability to have a malleable walltime for batch jobs. For times when suspending jobs is not viable and the draining of jobs on the system is required, the ability to run jobs as close as possible to the maintenance window is desirable. By specifying a minimum walltime and a maximum walltime, the batch scheduler will allow jobs to run if the minimum walltime can be started. This enables more efficient use of the system.

Results and Impact

By developing enhancements to the batch scheduler and InfiniBand software, the HECC systems team is able to maximizing the computing cycles available for NASA missions.

Researcher and Presenter at SC12:

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Demo 24

Live Demonstrations of 100-Gbps File Transfers Across LANs and WANs

Overview

Overcoming throughput bottlenecks in large file transfers over wide area networks (WANs) is critical to sharing data from NASA's Earth Science programs. The High-End Computer Network (HECN) Team at NASA Goddard Space Flight Center is investigating new high-performance servers, disk configurations, and 40- and 100-gigabit per second (Gbps) network interfaces to resolve these bottlenecks.

In cooperation with several partners, NASA will conduct live, real-time demonstrations of 100-Gbps file transfer experiments between the NASA exhibit (831) at SC12 and NASA Goddard in Greenbelt, MD, across 100-Gbps local and wide area networks.

Project Details

New technologies featured in these demonstrations include:

Intel Sandy Bridge EP processors and Supermicro X9DR3-F PCI Express Gen3-based motherboards with quad channels to memory

OCZ Vertex3 solid-state disks and LSI MegaRaid 9271 RAIDs

Hot Lava three-port 40-Gigabit Ethernet (GE) network interface cards

Prototype 100GE network interface cards developed by Acadia Optronics through a Department of Energy grant

100GE-capable switches and optical gear from Ciena, Brocade,

Infinera, ADVA, Fujitsu, Alcatel-Lucent, Arista, and possibly others

Results and Impact

Science research has transitioned from relying on two classic building blocks—theory and experimentation—to also using modeling and simulation. Increasingly, these techniques require massive amounts of data, which must be gathered, analyzed, stored, and transported among multiple sites worldwide.

The High-Performance Networking for Petascale Science Consortium was formed to investigate, evaluate, develop and demonstrate new techniques and methods to create services for transporting extremely large-scale data streams in support of petascale science at 100 Gbps. The consortium includes NASA Goddard, the International Center for Advanced Internet Research at Northwestern University, the Mid-Atlantic Crossroads, the Laboratory for Advanced Computing at the University of Chicago, Johns Hopkins University, the Naval Research Laboratory, the StarLight International/National Communications Exchange Facility, and the Metropolitan Research and Education Network. Consortium support comes from the ESnet Advanced Network Initiative, Ciena, and Sidera Networks. In addition to the above-mentioned collaborators, other key demonstration partners are SCinet, National LambdaRail, Internet2, Brocade, Fujitsu, cPacket, Arista, and Force10.

Role of High-End Computing Resources and Services

Using NASA Goddard's Science and Engineering Network (funded by the NASA Center for Climate Simulation) and several R&D WANs managed by our partners, the HECN Team achieved a throughput rate of approximately 60 Gbps when copying files over WANs at SC11. With new PCI Express Gen3 servers and processors, we expect to demonstrate nearly 100 Gbps cross-country WAN file transfers at SC12.

Researcher and Presenter at SC12:

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Demo 25

Untangling the Computing Landscape for Climate Simulations

Overview

The NASA Center for Climate Simulations (NCCS) at Goddard Space Flight Center (GSFC) supplies high performance computing and data services engineered to support climate simulations within the NASA Science Mission Directorate. Within the past few years, a number of technologies have emerged with the potential to change the landscape of high performance computing for climate simulations. The NCCS, along with its user community, has been exploring NVidia Graphical Processing Units (GPUs), Intel Many Integrated Core (MIC), Cloud Computing, Virtualized Infiniband, and have even begun to explore non-X86 processors such as the ARM or Atom. Making sense of these technologies and how to deploy them efficiently and effectively is not an easy challenge. This presentation will discuss the results from our exploration of a number of these advanced computing technologies and recommendations for how these can be deployed for high-end climate simulations.

Project Details

The NCCS high-end computing cluster, Discover, was augmented in October 2012 with Intel MIC processors. The upgrade consisted of 480 IBM iDataPlex nodes configured with Intel SandyBridge processors. Initially, the system has been configured with 240 Intel MIC processors with enough capacity to integrate more MIC processors in the future.

The NCCS has been exploring the use of cloud technologies and Virtualized Infiniband to support climate simulations within the Discover cluster. A test system of eight nodes was created out of representative components from the Discover cluster and configured with both native operating systems and virtual hosts. Representative kernel and application level benchmarks were run on this test cluster.

Also, the NCCS has begun exploring the use of non-X86 processors for potential use within climate simulations. This work is in the very beginning stages.

Results and Impact

The presentation will discuss a comparison of GPU to MIC processors and discuss how the NCCS is thinking about future deployments of these accelerator technologies. In addition, the presentation will show the kernel and benchmark results from the Virtualized IB test bed. Finally, the presentation will discuss future work on non-X86 processors and their potential to impact climate simulations. The overall impact of these technologies on high-end computing will be discussed.

Role of High-End Computing Resources and Services

The applications being run on Discover contribute to the overall scientific knowledge of climate change. Coupled with a robust and growing data analytic environment, the NCCS provides an environment in which large-scale climate models are executed, data is analyzed, and discoveries are made.

Researcher and Presenter at SC12:

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Demo 26

Simulating Galaxies and the Universe

Overview

According to the now-standard Lambda Cold Dark Matter (Λ CDM) theory, most of the universe is made up of invisible dark matter and dark energy. Bolshoi and BigBolshoi are the most accurate high-resolution Λ CDM simulations of the large-scale structure of the universe. Galaxy formation within the Λ CDM framework is so complicated that observation, theory, and simulation must work together in order to achieve understanding.

Project Details

We are using our state-of-the-art hydrodynamics plus N-body code hydroART to simulate hundreds of cosmological regions, each containing a large galaxy and many of dwarf and satellite galaxies.

The resulting large library of high-resolution cosmological simulations of galaxies forming in the standard Λ CDM cosmology, in different environments, and with different degrees of interaction provides an accurate sample of the observable universe.

Our Monte Carlo radiative-transfer code, Sunrise, enables us to make realistic images of the simulated galaxies in many wavebands at many times during each simulation, including the important effects of stellar evolution and dust. Directly comparing a statistical sample of hundreds of such “simulated observations” with HST, Spitzer, Herschel and other observations will help to clarify how galaxies form in different environments.

Since the resulting hundreds of thousands of images produced are far too many to be analyzed entirely by human eyes, we are currently developing techniques for human-computer interactions in order to classify these images using computer vision methods previously developed for other applications. Also 300,000 participants in the citizen science project GalaxyZoo are classifying real and simulated galaxies.

Results and Impact

Our simulations of galaxies forming in the standard Λ CDM cosmology are providing theoretical support for the interpretation of data gathered from NASA’s Hubble Space Telescope (HST) and other observatories, especially in connection with the largest HST program: Cosmic Assembly Near-IR Deep Extragalactic Legacy Survey (CANDELS).

Role of High-End Computing Resources and Services

The Columbia and Pleiades supercomputers at the NASA Advanced Supercomputing (NAS) Facility have been extremely helpful in running dissipationless simulations of large-scale structure evolution and the highest resolution (10-30 parsecs) hydrodynamic galaxy simulations. In addition, running our Sunrise “observations” of galaxy simulations on NASA’s new 64 Pleiades graphic processor unit (GPU) nodes is allowing a factor of ten speedup. Lastly, collaboration with NAS visualization experts has been crucial to visualizing and interpreting the results of these simulations, and in generating materials for the purposes of public outreach.

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Demo 27

The Mysterious Origin of Stellar Masses

Overview

Most stars have a mass similar to that of our Sun or a few times smaller. Extreme cases, 100 times less or more massive than the Sun, are much more rare. The classical theory of gravitational instability cannot explain this characteristic stellar mass, nor the wide spread of values between the extreme cases.

The key to this problem is the turbulent nature of stellar nurseries, cold clouds formed primarily of molecular hydrogen, characterized by violent internal motions many times the

speed of sound. Through the effect of strong shocks, this supersonic turbulence results in a complex network of dense filaments, where the observed stellar masses can be assembled. Using NASA's fastest supercomputer, we carried out the largest simulations to date of star-forming clouds, capable of capturing the full range of stellar masses.

Project Details

We use a heavily modified version of the public adaptive-mesh-refinement code Ramses, allowing us to run effectively on a large fraction of the NASA/Ames Pleiades supercomputer. By focusing the computational resources onto the densest regions, with the adaptive-mesh-refinement method, we achieve a maximum resolution equivalent to that of a uniform grid with 131,0723 computational cells.

Our simulations yield the full range of stellar masses, from a few percent of a solar mass, to almost one hundred solar masses. They also reproduce the observed probability distribution of stellar masses.

Results and Impact

Our simulations allow us to test theoretical models of star formation that are necessary to understand the formation of galaxies. They elucidate the process that assembles the mass of stars and shed new light onto the early phases of star and planet formation.

Each simulation results in thousands of stars, providing very large statistical samples of initial conditions for protoplanetary discs around normal stars and gas accretion around massive stars. Such simulated initial conditions can be used to make predictions and interpretations for observations with space and ground based observatories.

Role of High-End Computing Resources and Services

Thanks to the NASA/Ames Pleiades supercomputer, we have achieved the largest star-formation simulation to date, using thousands of processors. NASA's large shared-memory machines, such as Bridge3 and Bridge4, and huge online disk storage have provided us with a powerful environment for data analysis, crucial to extract scientific results from the simulations.

Deeper insight on the structure and evolution of the modeled star-forming regions was also provided by graphic visualizations carried out by the visualization team at NASA Ames.

Researcher and Presenter at SC12:

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Demo 28

Hot-Plasma Geysers on the Sun

Overview

The Sun is covered by geyser-like plasma eruptions ("spicules") which provide mass and energy to the million-degree corona and to the solar wind affecting the Earth's space environment. Due to the small-scale structure and fast dynamics these eruptions were not well resolved in observations, and their origin was not known. Realistic 3D radiative magneto-hydrodynamics (MHD) simulations allowed us to reproduce these eruptions,

investigate their structure, and uncover the driving mechanism hidden in the turbulent convection zone below the visible surface of the Sun.

Project Details

The simulation domain includes the upper convective boundary layer, photosphere and chromosphere of the Sun. The mathematical model is based on first physical principles, and employs the Large-Eddy Simulation (LES) approach of MHD turbulence simulations and a multi-group approximation for radiation transfer. The simulations utilize a parallel "SolarBox" code developed at NASA/Ames. The code runs very efficiently on large number (1000-4000) of processors.

Driven by the energy flux from the energy-generating core of the Sun the turbulent convection forms granulation cells with high-speed downflows in the intergranular lanes. The overturning and shearing flows below the solar surface form compact self-organized turbulent vortex tubes with high-speed swirling flow. The vortex tubes are concentrated in the intergranular lanes. They interact with surrounding magnetic field twisting magnetic field lines. Due to the pressure excess accumulated in the low atmospheric layers the magnetized vortex tubes erupt in a manner similar to geyser eruptions.

Results and Impact

The realistic simulation revealed that the ubiquitous flow eruptions on the Sun are produced by self-organized magnetized vortex tubes generated by turbulent convection below the visible surface of the Sun. These results allow us to better understand the mass and energy flowing from the Sun into the heliosphere and the Earth's space environment, and use this knowledge for interpretation of data from the Solar Dynamics Observatory (SDO), Hinode and IRIS missions, and for developing physics-based models of the solar dynamics and activity.

Role of High-End Computing Resources and Services

The realistic radiative 3D MHD numerical simulations require massive computational resources. These tasks were accomplished using the Pleiades supercomputer system at the NASA Ames Advanced Supercomputing (NAS) Division, which demonstrated a highly efficient performance for massive parallel computations. The 3D visualization (with the support of Tim Sandstrom and Chris Henze, NASA/NAS) greatly contributed to the success of this project.

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Demo 29

Turbulent Life of Kepler Stars

Overview

NASA's Kepler mission has discovered a whole new world of extra-terrestrial planets and variable stars. It was particularly surprising that the stars with convective envelopes much

thinner than on the Sun show significant fluctuations in brightness, and also strong stochastic acoustic oscillations of the solar type. Because of the large distance the surface of these stars cannot be resolved in observations. Thus, numerical simulations is the only way to learn about the structure of their surface and dynamics. The simulations provided the first detailed view of the turbulent surface of the planet-hosting stars that are more massive than the Sun, and allowed us to discover the mechanisms of the stellar acoustic emission.

Project Details

The stellar turbulence simulations were performed using 3D radiative hydrodynamics code "StellarBox" developed at NASA/Ames by Alan Wray and Nagi Mansour. The code employs high-order Pade finite-difference scheme and LES (Large-Eddy Simulation) subgrid-scale models for accurate description of the stellar turbulence and acoustics. The simulations were performed for several Kepler-target stars in the mass range from 1.05 to 1.7 solar masses, using the standard hydrostatic stellar evolutionary models for the initial conditions. The simulations were performed on the Pleiades system using 1,000-2,000 processors.

Results and Impact

The simulations revealed that the surface convective layers on the stars are much more dynamic and turbulent than on the Sun. Because of their higher luminosity, the turbulent energy transport is substantially greater driving supersonic turbulence and strong acoustic emission. The stellar granulation cells are bigger than the solar granulation, and often penetrated by high-speed plumes rarely seen on the Sun. The most interesting phenomenon is formation of large-scale turbulent vortices on the star's surface, which generate acoustic waves. These waves form global resonant acoustic modes discovered for this type of stars by the Kepler mission. The strong turbulence and acoustic emission found in the simulations are likely to energize the stellar wind leading have profound effects on the extra-terrestrial planets.

Role of High-End Computing Resources and Services

The radiative hydrodynamics numerical simulations of the stellar turbulent dynamics were performed by Dr Irina Kitiashvili (Stanford) using the Pleiades supercomputer system at the NASA Ames Advanced Supercomputing (NAS) Division, which demonstrated a highly efficient performance for massive parallel computations. The 3D visualization was created by Tim Sandstrom and Chris Henze (NASA/NAS).

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Demo 30 **Modeling Weather on the Sun**

Overview

The Sun's weather is modeled (in a similar fashion to Earth's weather) by numerically solving the conservation equations for mass, momentum and energy plus the induction equation for the magnetic field. This allows us to study the magneto-dynamics of the solar surface, especially the emergence of magnetic fields in both the quiet Sun and active regions. It is magnetic fields emerging through the solar surface that control the heating of the solar chromosphere and corona and the eruption of flares and coronal mass ejections.

Project Details

We simulate magneto-convection near the solar surface using the 3D, compressible, magneto-hydrodynamic, finite difference STAGGER code in a Cartesian grid with the vertical coordinate stretched for finer resolution near the visible surface. A tabular real gas equation of state is used including ionization and excitation of hydrogen, helium and other abundant elements. Radiative heating and cooling is calculated by solving the non-grey radiation transfer equation with four opacity and emissivity groups using long characteristics.

Uniform, untwisted, horizontal, one kilogauss magnetic field is advected into the domain through the bottom boundary at 20 Mm depth (10% of the geometric depth of the solar convection zone but 2/3 of its density scale heights) in order to represent the effects of dynamo action in the deeper layers.

Results and Impact

Magneto-convection, acting on large-scale dynamo produced fields from the lower convection zone produces a hierarchy of magnetic loops with smaller ones as serpentine features on larger loops.

Large loop complexes emerge through the solar surface as active regions. First, mixed polarity fields emerge as small, granule sized loops over enlarged, elongated granules. Then opposite polarity fields collect into separate, unipolar concentrations driven by the underlying large scale field structure to form the active region.

Validity of inversions of Stokes profiles to obtain 3D magnetic fields is being evaluated by comparing inversions of simulated Stokes spectra with actual magnetic fields in the calculations. Inversions of weak fields (< 100-200 G) are found to be unreliable due to the complex vertical structure of the magnetic and velocity fields and exacerbated by the limited resolution of the telescopes.

These results enable us to understand and evaluate the results from NASA missions such as the Solar Dynamics Observatory and Hinode.

Role of High-End Computing Resources and Services

These simulations require several million processor hours on the NASA Pleiades supercomputer, which takes months of wall time even running on thousands of cores. They would be impossible without these resources.

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Demo 31

Weather on Mars: The Meteorology of Gale Crater

Overview

On August 5th, 2012, the Mars Science Laboratory 'Curiosity' rover landed in Gale Crater near the martian equator. The chosen landing site was deemed both of high scientific value as well as safe for entry, descent and landing (EDL) and long-term surface operations. To demonstrate safe conditions in the martian atmosphere over Gale Crater, a long-term investigation into the meteorology around the site was undertaken.

Project Details

As a way of understanding the local meteorology at Gale Crater, we employed the Mars Weather Research and Forecasting (MarsWRF) general circulation model (GCM) to simulate atmospheric behavior at various times of year over Gale Crater.

The flexible nature of MarsWRF allows us to use the same model architecture from the largest, global scales down to very fine resolution grids that capture the local behavior within the crater itself, including winds, temperature and pressure. Local topography and surface properties are obtained from orbital observations from previous spacecraft. These results can be compared to data obtained by the Curiosity rover during its mission to evaluate the efficacy of such GCMs to serve a predictive role in understanding local meteorology. Additional investigations, using a thicker, warmer atmosphere representative of early conditions on Mars can be run to explore the possibility of liquid water existing for long periods in this location much early in Mars' history.

Results and Impact

Results with the MarsWRF GCM demonstrate a strong diurnal component to the wind field inside Gale Crater, with largely upslope winds (northerlies at the Curiosity landing site) during daytime and downslope winds (southerlies) at night. This is consistent with topographically driven circulation and is similar to behavior seen along the flanks of terrestrial topographic features.

The results of this work, and, more specifically, identification of those areas in which the GCM does not match well to the observed meteorology by Curiosity will improve predictions for future landed missions on Mars and reduce overall system margins, which will have the effect of reducing mission cost, mass and complexity.

Role of High-End Computing Resources and Services

Use of the 'Cosmos' supercomputer at JPL for the general circulation modeling, along with the availability of large, long-term storage of model output were invaluable resources for achieving these objectives. A typical 30-day simulation, with four embedded model nests (from global down to local scale) takes about three days on 16 CPUs.

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Demo 32

Enhancing Performance of NASA's High-End Computing Applications

Overview

The Application Performance and Productivity (APP) group of the High-End Computing Capability (HECC) Project at the NASA Advanced Supercomputing facility has three key activities: enhancing performance of high-end computing applications, leveraging software technologies to improve user productivity, and characterizing performance of current and future architectures.

Project Details

Recent application optimization efforts boosted the performance of several user codes, including introducing OpenMP in two codes, Satellite Data Simulation Unit (SDSU) code and a solar acoustic computational code (A_SH_B_WAVES) to gain a performance boost of 8x and 2.7x respectively; and improving the IO performance of the Goddard Cumulus Ensemble (GCE) code, allowing it to scale up to 4096 cores.

Results and Impact

The group also enhanced user productivity and system efficiency in several ways including developing a methodology to package hundreds to thousands of serial (UCLA-Aurora, JPL-L2_FP, GRC-SWBLI) or parallel (ARC-Aero CFD) simulations in a single batch job; creating a tool, lumber, to facilitate rapid analysis of individual job failures and system-wide issues by mining for error patterns in log messages; and developing a methodology, unit, to detect a large class of uninitialized floating-point variables, which are undetected by standard compiler options.

Role of High-End Computing Resources and Services

The APP group uses a suite of NASA-relevant codes regularly to characterize performance of new high-performance computing architectures, including new Intel Xeon-based systems, NVIDIA GPUs and Cloud offerings. The group helped develop a knowledge base approach for user documentation and initiated user training through regular webinars.

Researchers and Presenters at SC12:

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Demo 33

Designing Curiosity's Perfect Landing on Mars

Overview

At 10:32 pm (PDT) on August 5th, 2012 millions of people from around the world watched as the Curiosity rover gently touched down onto the floor of Gale Crater next to a six-kilometer mountain. Five hundred-thousand lines of the most sophisticated interplanetary-autonomous-autopilot code brought the spacecraft down from a speed of 13,000 kilometers per hour (km/h) at the top of the Martian atmosphere to 0 km/h on the surface of Mars in just seven minutes. NASA's Jet Propulsion Laboratory (JPL) used its unique entry, descent and landing (EDL) knowledge combined with thousands of CPU hours from several

Beowulf clusters to orchestrate the sequence of events that successfully placed this 2,000-pound rover onto the surface of Mars.

Project Details

The Jet Propulsion Laboratory built the biggest robotic exploration rover yet, which is carrying 10 times more payload in scientific instruments than the Mars Exploration Rovers. Curiosity is the most comprehensive Martian geologist to rove the red planet. It carries 17 different cameras, 4 spectrometers, 2 radiation detectors, an environment sensor, and an atmospheric sensor. A radioisotope thermoelectric generator (RTG) that produces 110 watts powers the rover.

Engineers at JPL sent Curiosity on a nine-month journey across 350,000,000 miles for a precision landing on Mars. JPL designed the spacecraft to steer itself using a series of S-curves for a guided entry through Mars' atmosphere. Three minutes from touchdown the spacecraft parachute-decelerated to about 200 mph in an atmosphere that is 100 times thinner than that of earth. Finally, the spacecraft used a series of retro rockets and a sky crane to complete its precision landing sequence touching down inside the smallest ever Martian landing ellipse.

Results and Impact

Curiosity's overarching science objective is to evaluate whether Mars has ever had or still has the necessary environmental conditions for life. Scientists believe that the alluvial fan on the floor of Gale Crater may have been created by water-carried sediments and may hold the key to answering the question about life on Mars. Scientists also believe that Mount Sharp's layered formation may contain minerals formed in water that are the building blocks of life. Curiosity has a long journey of discovery ahead of it, but it has already captivated the hearts of scientists, engineers, and many others through its revolutionary achievements in science and technology.

Role of High-End Computing Resources and Services

Sixteen months ago, JPL's Entry, Descent, and Landing team (EDL) began working with JPL's Supercomputing team to create a fully customized supercomputing environment necessary to run the complex guided entry simulations. The Supercomputing team used version-control and automated build techniques to allow the team to recreate any version of the customized environment.

The Monte Carlo simulation used for Curiosity ran a series of high-fidelity trajectory integrations that had a unique set of inputs for each embarrassingly parallel simulation. A precision landing with guided entry required each Monte Carlo simulation to have 8,001 separate trajectory integrations, requiring 90 minutes of run-time for each simulation. JPL's Supercomputing capabilities allowed the EDL team to dramatically reduce the risk in landing at Gale Crater. "Having that resource available made it very nice for us", stated Paul Burkhart from JPL EDL Guidance and Control Systems.

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Demo 34

The Search Continues: Kepler's Quest for Habitable Earth-Sized Planets

Kepler is NASA's first mission capable of finding Earth-size and smaller planets around other stars. Launched in March of 2009, the *Kepler* spacecraft has been continuously monitoring over 150,000 stars in the constellations of Cygnus and Lyra, watching for the periodic dimming of the stars that may indicate the presence of an exoplanet passing in front of the star from the perspective of our own solar system.

Project Details

Kepler's sole instrument is a specially designed photometer with a 0.95-meter aperture telescope. It has a very large field of view for an astronomical telescope — 115 square degrees, which is comparable to the area of your hand held at arm's length. It needs that large a field in order to observe the necessary large number of stars.

Kepler's photometer contains the largest digital camera to ever fly in space, consisting of 42 charge-coupled devices (CCDs) for a total of nearly 95 megapixels. Pixels of interest are downlinked once a month and transferred to the *Kepler* Science Operations Center (SOC) at NASA Ames Research Center in California. Here the pixels are calibrated, combined to form light curves, corrected for systematic errors introduced by the instrument, then searched for the signatures of transiting planets.

Results and Impact

As of February 2012, the *Kepler* team has found 2321 planetary candidates circling 1790 host stars (with 77 confirmed to be planets by other means). Roughly a third or more are in multiple-planet systems. Some of these systems also involve planetary candidates orbiting binary star systems (circumbinary planets). Hundreds of candidates have now been found that are Earth-sized although not in the habitable zone of their respective stars. Several planetary candidates however do occupy the habitable zone, although they are not Earth-sized. As the mission continues, additional longer period candidates continue to be found and trends suggest that we should start filling in the most interesting portion of parameter space, namely, the habitable zone Earth-size planets.

Role of High-End Computing Resources and Services

We have successfully ported the most computationally expensive portions of the pipeline (Pre-Search Data Conditioning, Transiting Planet Search, and Data Validation modules) to the Pleiades supercomputer, and have demonstrated near perfect (linear) strong scaling up to 75,000 processors. We have also developed software that automatically copies data between the *Kepler* SOC and Pleiades so that we can run the less expensive parts of the pipeline in the SOC, while running the most expensive parts on Pleiades, in a manner that is transparent to the operators. The addition of features to other portions of the data processing pipeline has necessitated their migration to the supercomputer as well. That work is currently underway. Employing the supercomputer will allow us to realize the benefit of our code improvements on a much shorter time-scale than we currently operate under due to our locally limited computing resources. This will further benefit the general public as well since, beginning in December, both pipeline results as well as data will become available through NExSci as we continue on into *Kepler*'s Extended Mission.

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