National Aeronautics and Space Administration

# NASA Advanced Computing Environment for Science & Engineering

Dr. Rupak Biswas

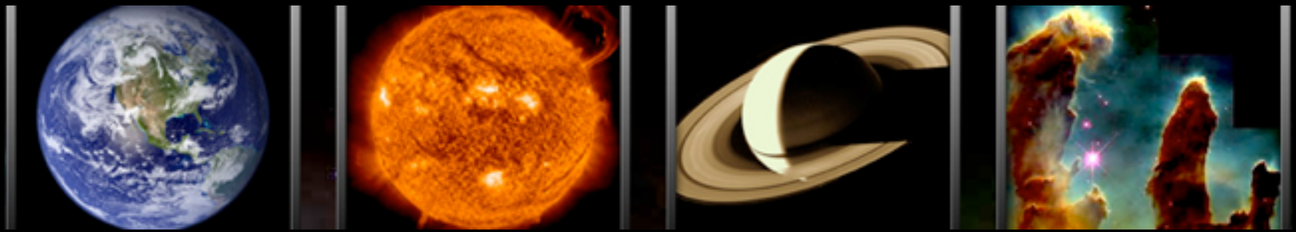
*Deputy Director, Exploration Technology Directorate*
*Manager, High End Computing Capability (HECC) Project*

NASA Ames Research Center, Moffett Field, Calif., USA

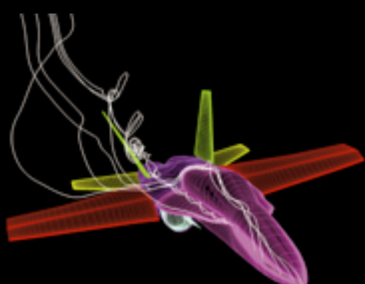
*High Performance Computing Day, VirginiaTech, Blacksburg, VA*
*6 April 2015*

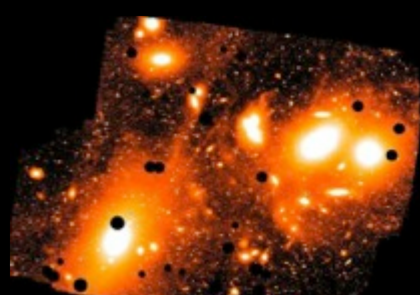
# NASA Overview: Mission Directorates

- **Vision:** *To reach for new heights and reveal the unknown so that what we do and learn will benefit all humankind*
- **Mission:** *To pioneer the future in space exploration, scientific discovery, and aeronautics research*
- **Aeronautics Research (ARMD):** Pioneer and prove new flight technologies for safer, more secure, efficient, and environmentally friendly air transportation
- **Human Exploration and Operations (HEOMD):** Focus on ISS operations; and develop new spacecraft and other capabilities for affordable, sustainable exploration beyond low Earth orbit
- **Science (SCMD):** Explore the Earth, solar system, and universe beyond; chart best route for discovery; and reap the benefits of Earth and space exploration for society
- **Space Technology (STMD):** Rapidly develop, demonstrate, and infuse revolutionary, high-payoff technologies through collaborative partnerships, expanding the boundaries of aerospace enterprise



# NASA Overview: Centers & Facilities

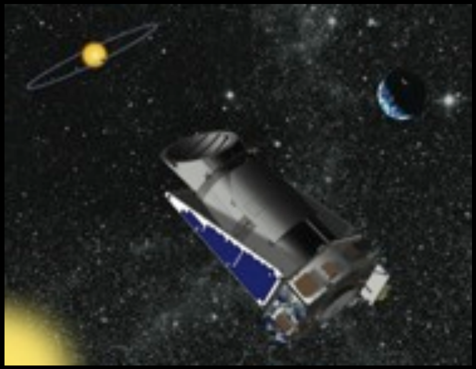





# Need for Advanced Computing

## Enables modeling, simulation, analysis, and decision-making

- Digital experiments and physical experiments are tradable
- Physical systems and live tests are generally expensive & dangerous (e.g., extreme environments), require long wait times, and offer limited sensor data
- NASA collects and curates vast amounts of observational science data that require extensive analysis and innovative analytics to advance our understanding

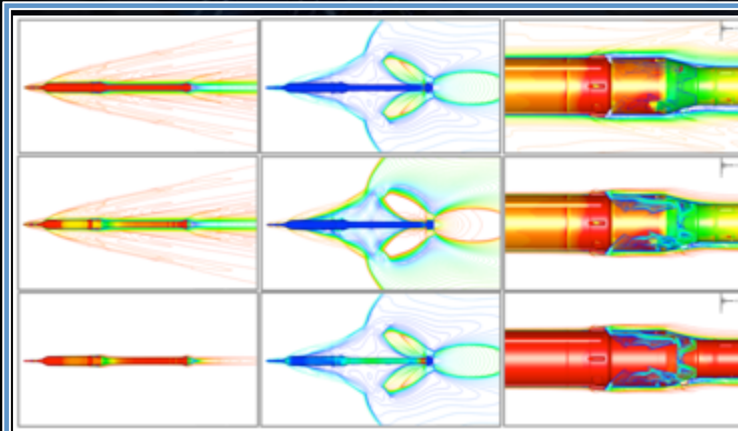



- Decades of exponentially advancing computing technology has enabled dramatic improvements in cost, speed, and accuracy – in addition to providing a predictive capability
- Many problems pose extremely difficult combinatorial optimization challenges that can only be solved accurately using advanced technologies such as quantum computing
- NASA's goals in aeronautics, Earth and space sciences, and human and robotic exploration all require orders-of-magnitude increase in computing capability to enhance accuracy, reduce cost, mitigate risk, accelerate R&D, and heighten societal impact

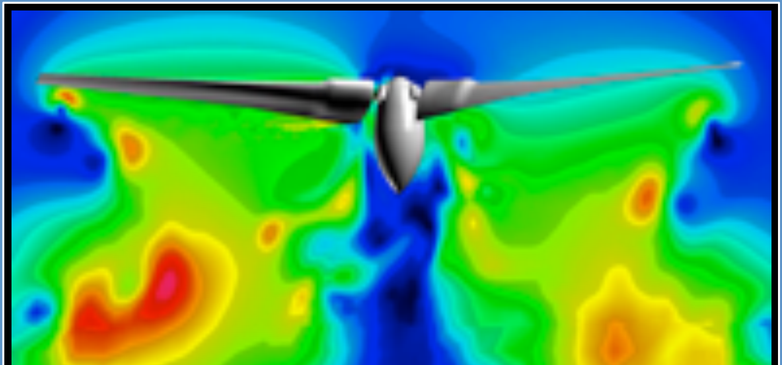
# Advanced Computing Environment

# NASA's Diverse HPC Requirements

- Engineering requires HPC resources that can process large ensembles of moderate-scale computations to efficiently explore design space ***(high throughput / capacity)***
- Research requires HPC resources that can handle high-fidelity long-running large-scale computations to advance theoretical understanding ***(leadership / capability)***

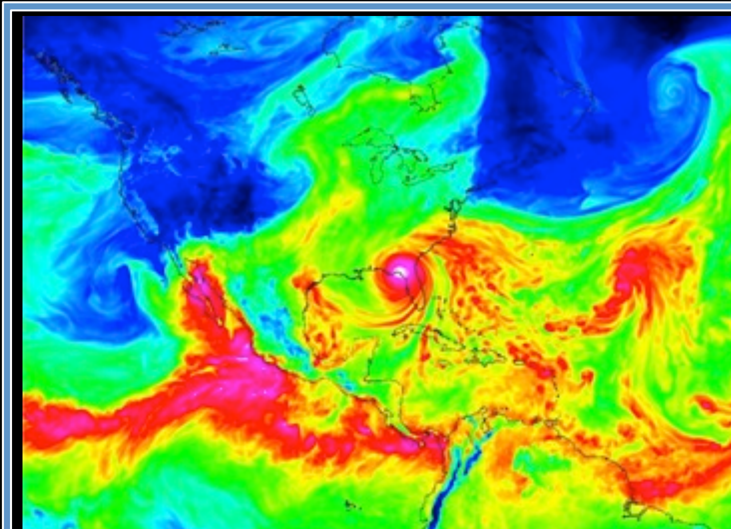


Aerodynamic database generation



Rotary wing unsteady aerodynamics

- Time-sensitive mission-critical applications require HPC resources on demand ***(high availability / maintain readiness)***



Real-time hurricane prediction

# Balanced HPC Environment

## Computing Systems

- *Pleiades:* 185K-core SGI Altix ICE with multiple generations of Intel Xeon (2 racks GPU-enhanced); 3.6 PF peak
- *Endeavour:* Two SGI UV2000 nodes with 2 and 4 TB shared memory SSI via NUMALink-6
- *Maia* and *Mira:* Two testbeds (SGI and Cray) with 60-core Intel Phi accelerators
- *hyperwall:* 128-node GPU cluster for large-scale rendering and concurrent visualization

## Data Storage

- 20 PB of RAID over several Lustre filesystems
- 115 PB of tape archive

## Networks

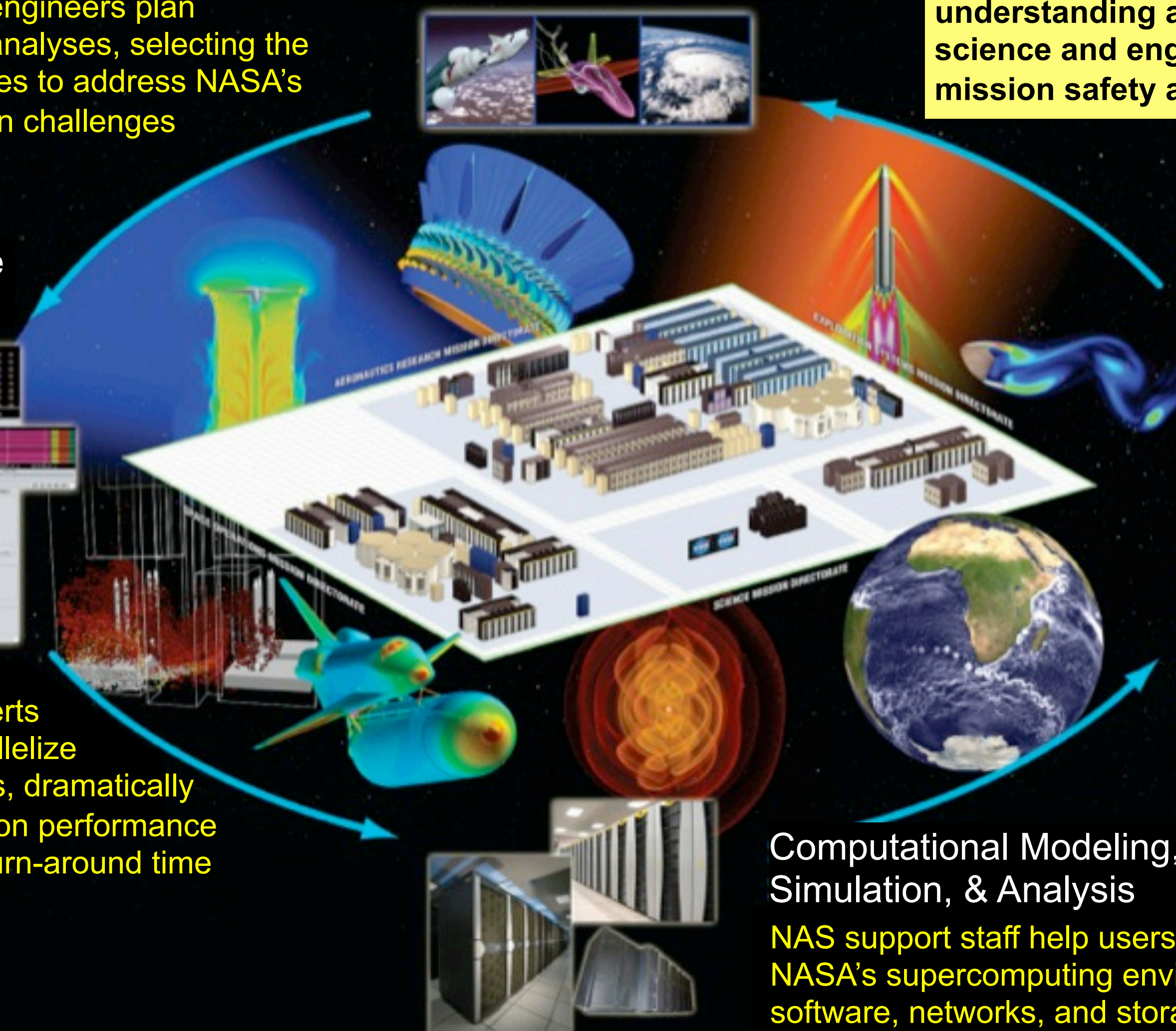
- InfiniBand interconnect for Pleiades in partial hypercube topology; connects all other HPC components as well
- 10 Gb/s external peering

# Integrated Spiral Support Services

NASA Mission Challenges

**Outcome: Dramatically enhanced understanding and insight, accelerated science and engineering, and increased mission safety and performance**

Scientists and engineers plan computational analyses, selecting the best-suited codes to address NASA's complex mission challenges



Performance Optimization

NAS software experts utilize tools to parallelize and optimize codes, dramatically increasing simulation performance while decreasing turn-around time

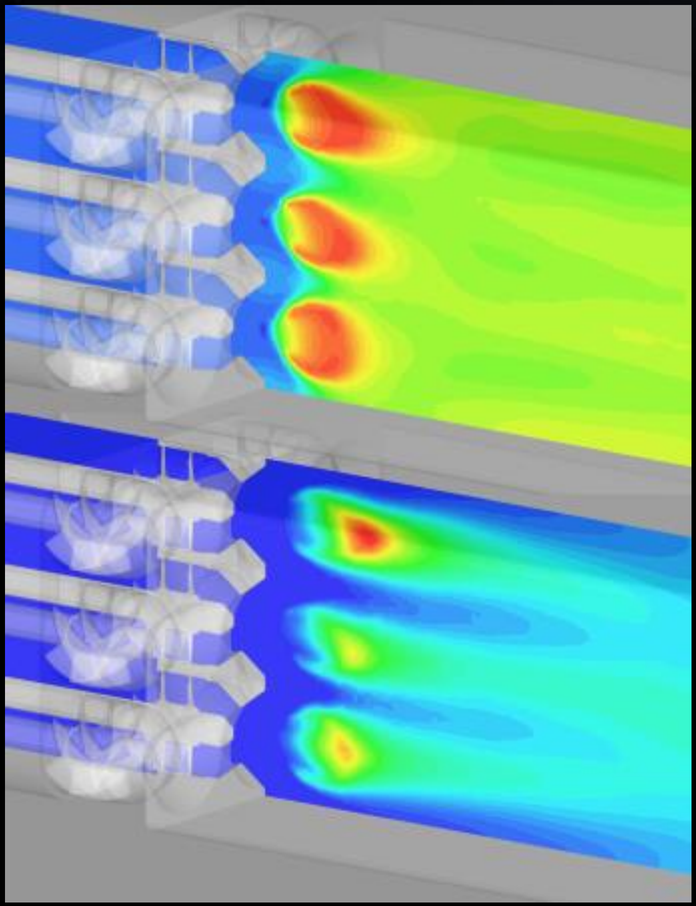
Data Analysis and Visualization

NAS visualization experts apply advanced data analysis and rendering techniques to help users explore and understand large, complex computational results

Computational Modeling, Simulation, & Analysis

NAS support staff help users to productively utilize NASA's supercomputing environment (hardware, software, networks, and storage) to rapidly solve large computational problems

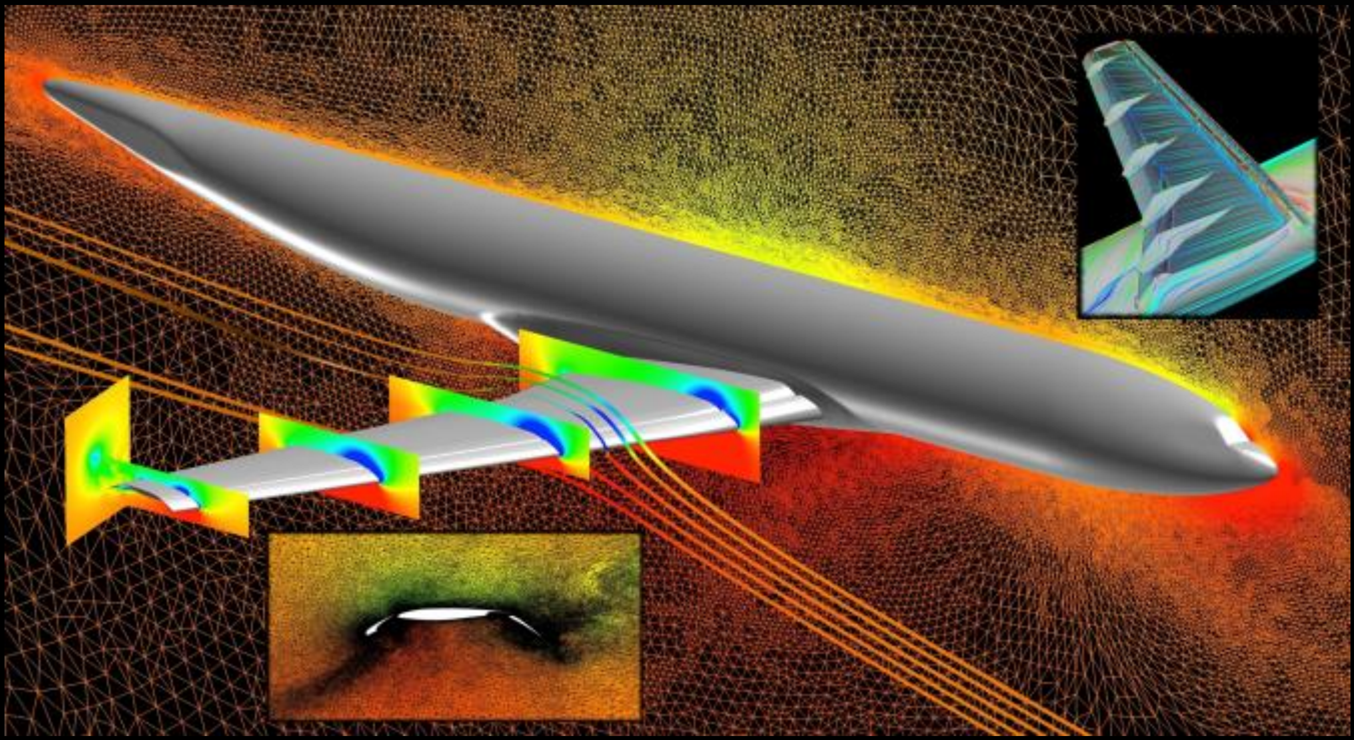
# Aeronautics



Clean Aircraft Engines

*Jeff Moder and Kumud Ajmani (GRC)*

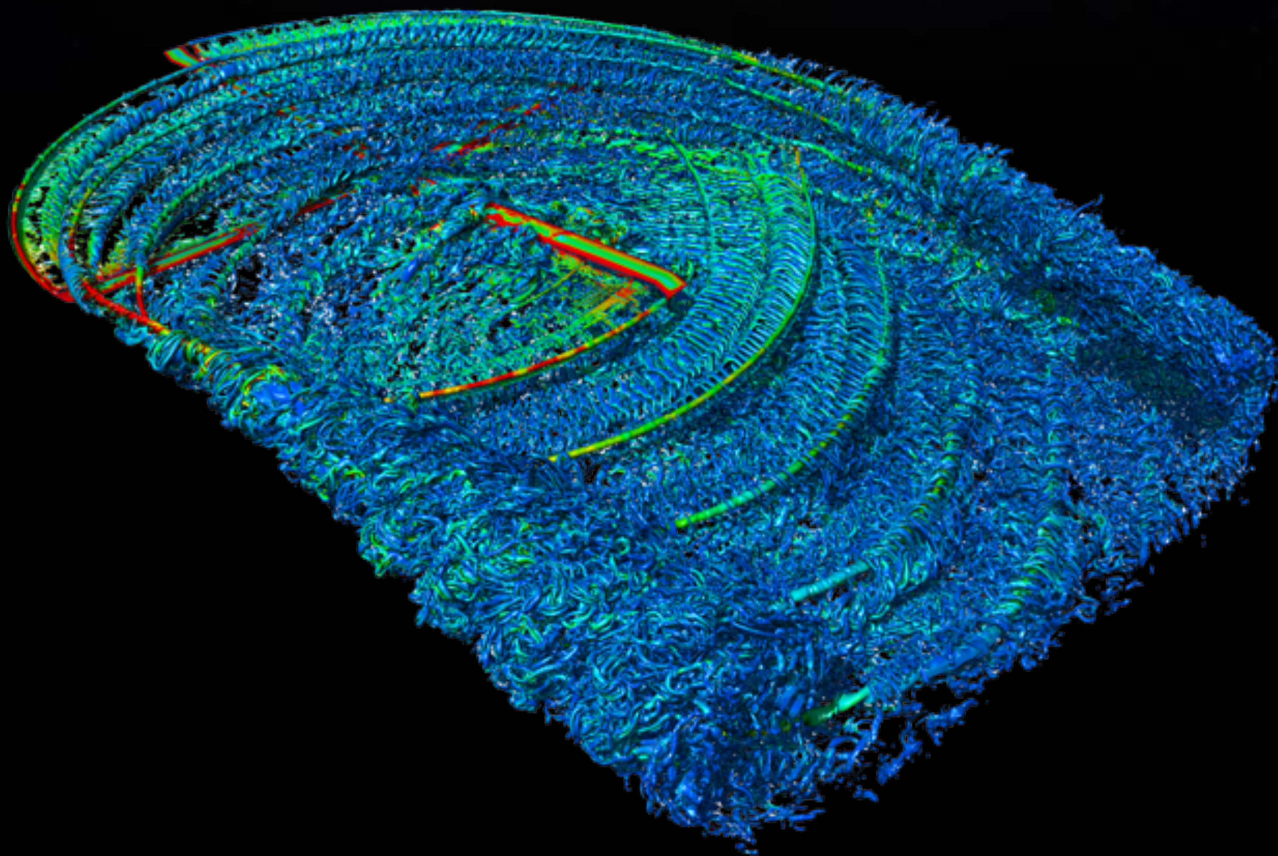
# Aeronautics



Complex Aerospace Vehicles

*Eric Nielsen and Dana Hammond (LaRC)*

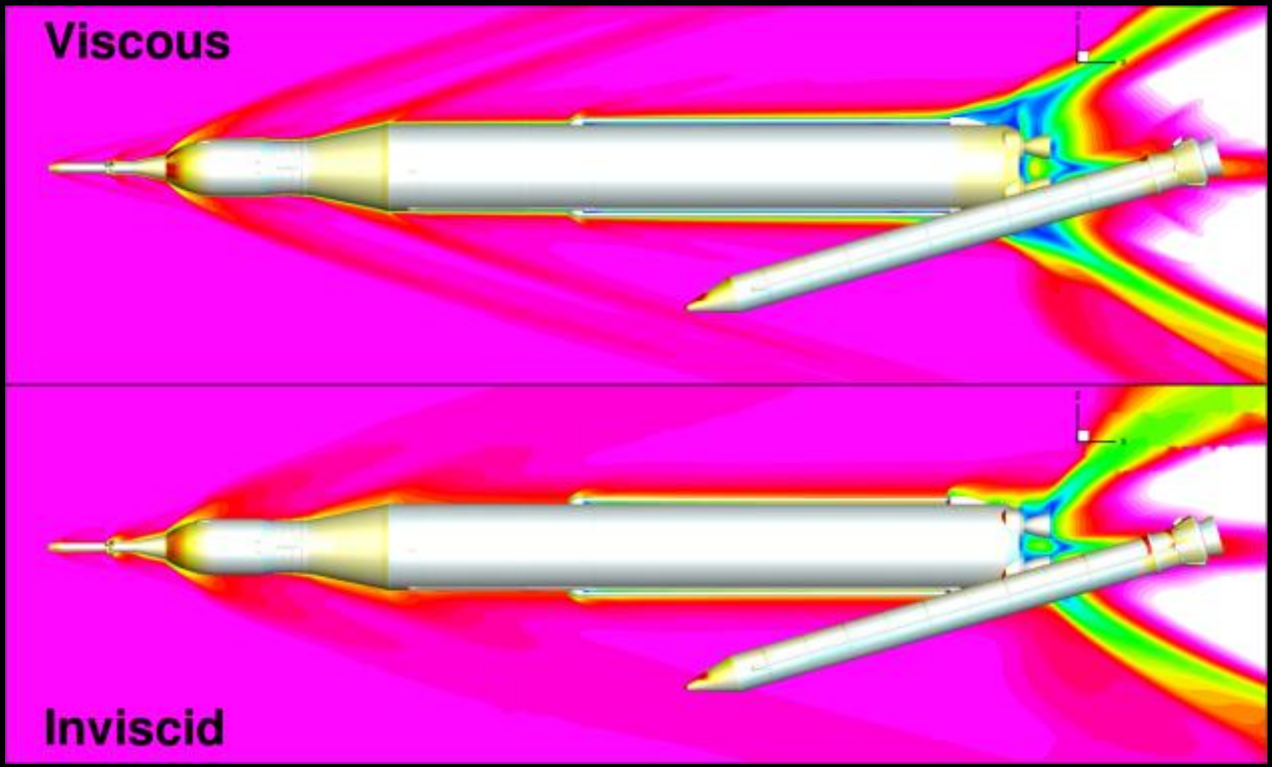
# Aeronautics



Advanced Rotorcraft Simulations

*Neal Chaderjian and Jasim Ahmad (ARC)*

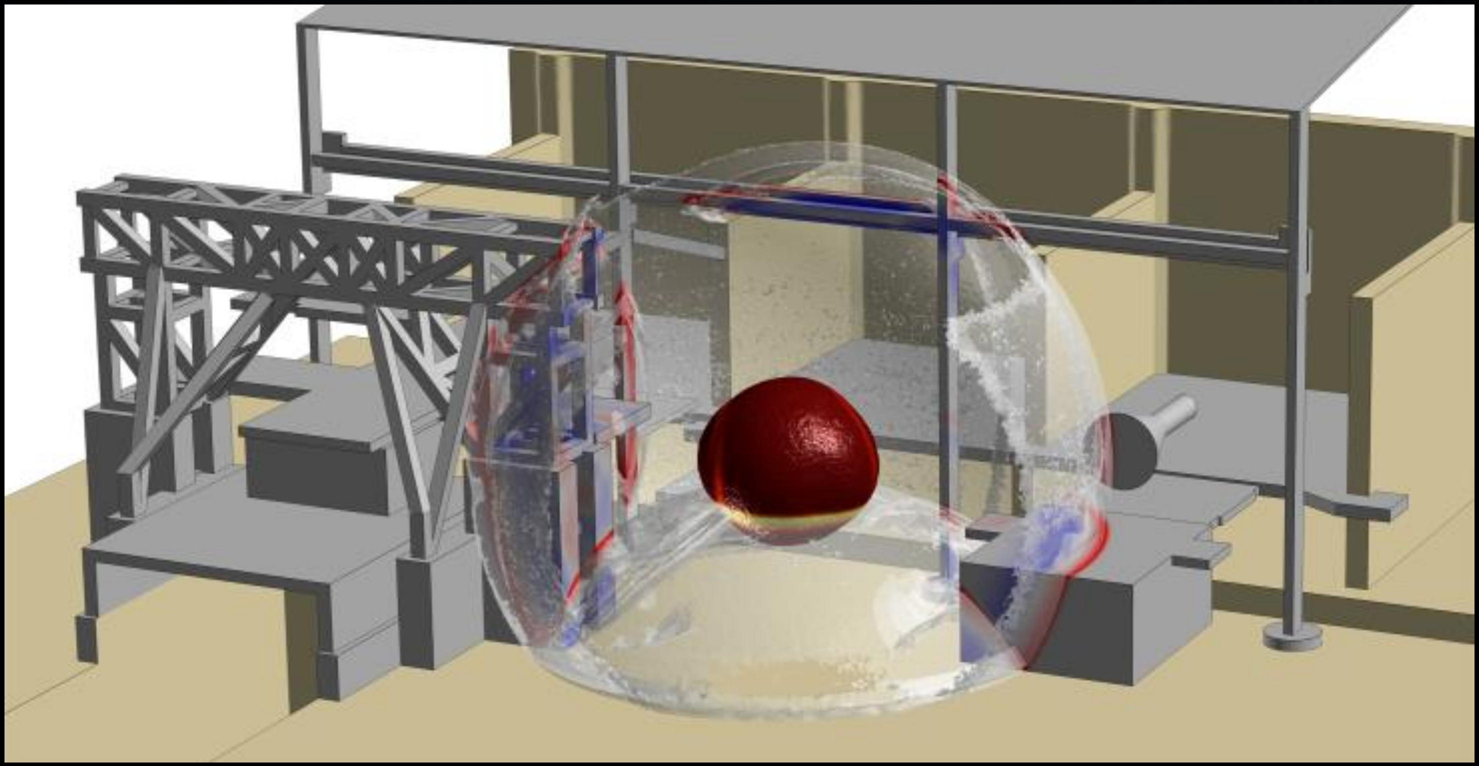
# Space Exploration




Launch Vehicle Design

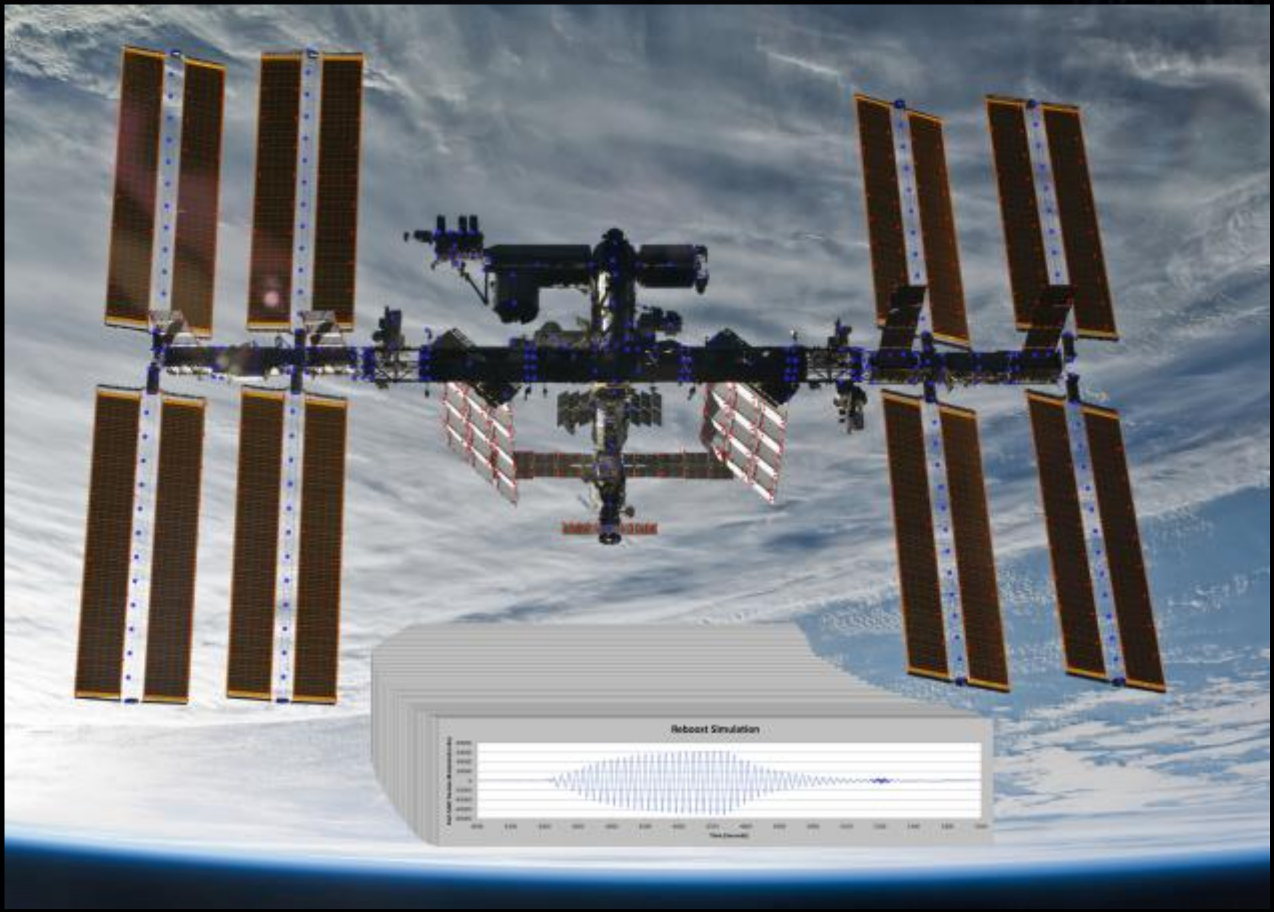
*Cetin Kiris (ARC)*

# Space Exploration



Safety Risk Mitigation
*Brandon Williams (MSFC)*

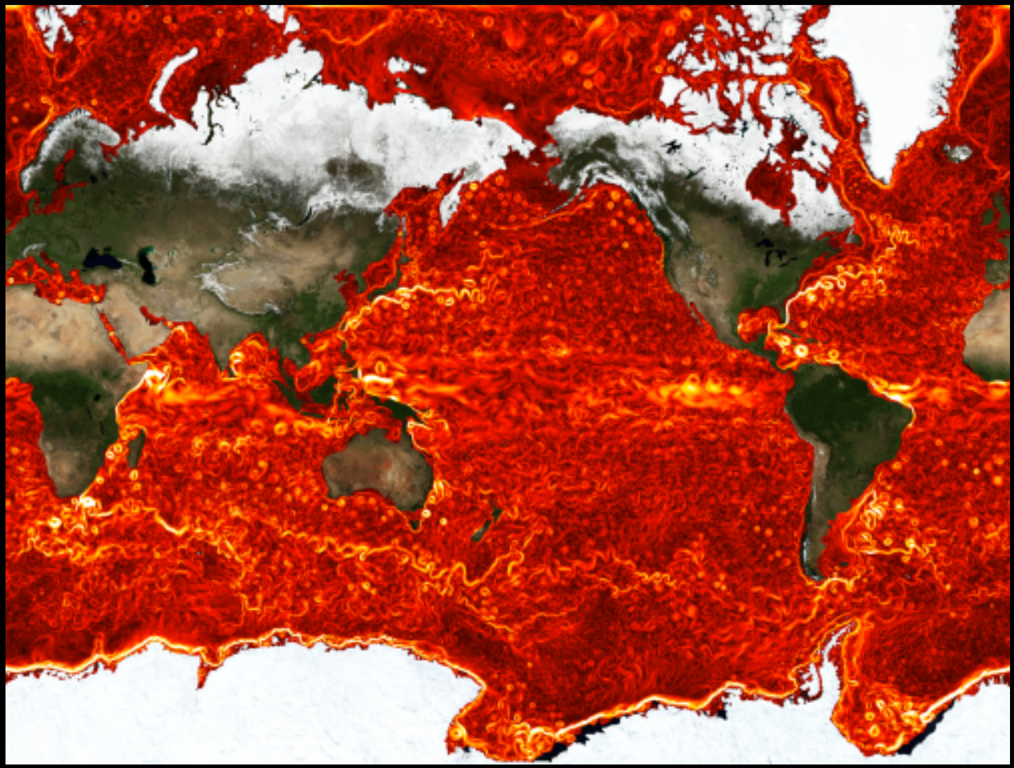
# Space Exploration




ISS Structural Analysis

*Michael Grygier (JSC)*

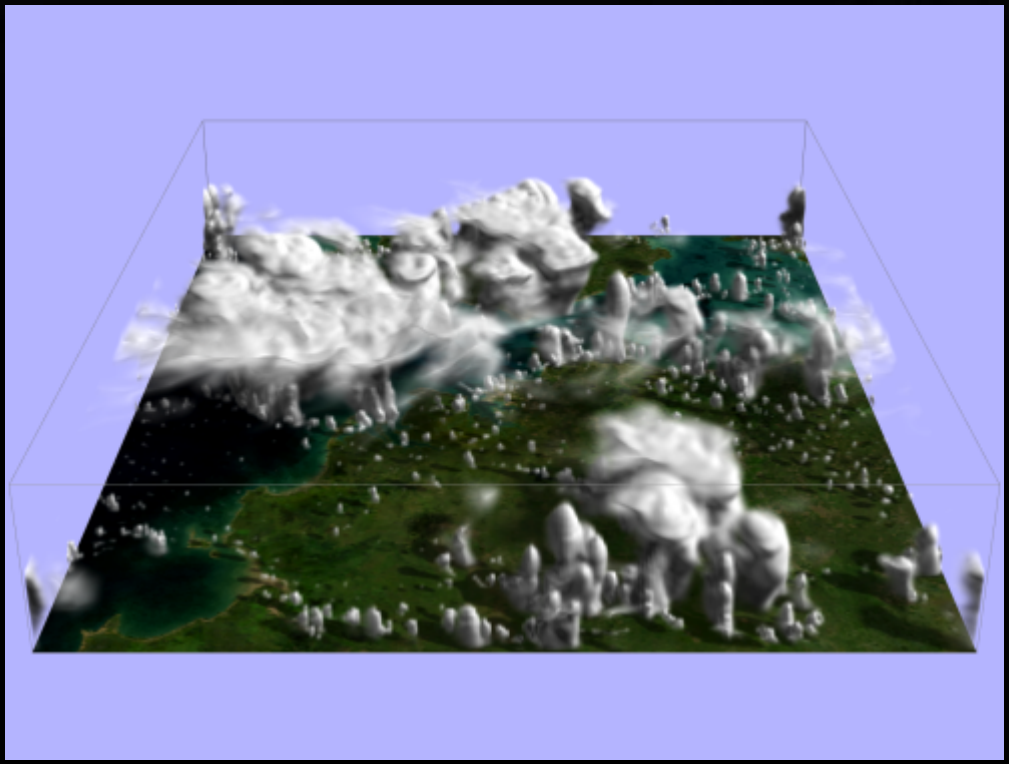
# Our Planet



Global Ocean Reconstructions

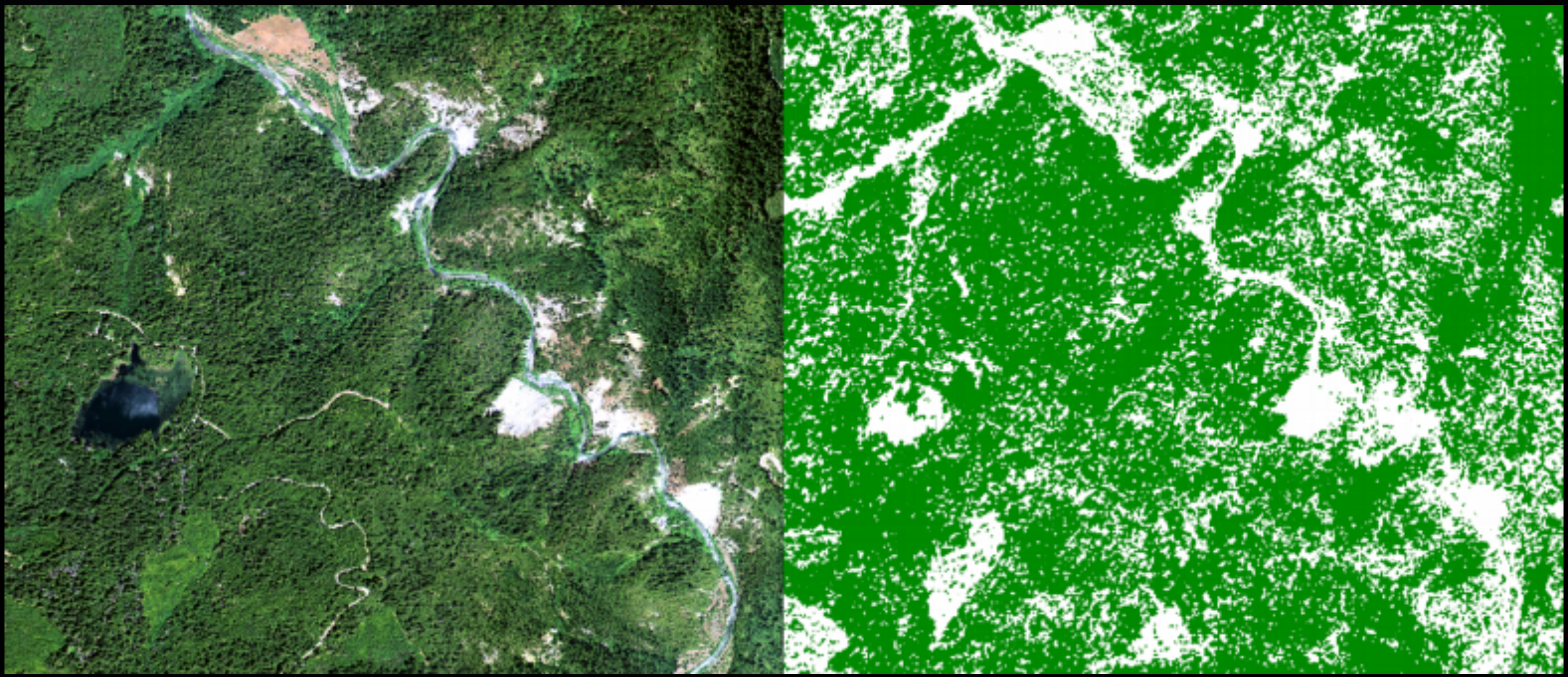
*Chris Hill (MIT) and Dimitris Menemenlis (JPL)*

# Our Planet



Hurricane Modeling & Prediction
*Xiaowen Li and Wei-Kuo Tao (GSFC)*

# Our Planet



Forest Cover Analysis

*Petr Votava and Andrew Michaelis (ARC)*

# Accelerator Technologies

## Significant performance potential for science and engineering applications

- Execute many threads simultaneously at relatively lower power

## Two primary viable options

- *Nvidia GPGPU:* Did not get much traction within NASA
- *Intel MIC:* Code commonality across host and co-processor was initially promising

## Intel Xeon Phi evaluation

- 128 nodes, each with 2 Sandy Bridge and 2 Phi
- Examine performance in four different execution modes: Native Host, Off-load, Symmetric, Native MIC
- *Micro-kernel benchmarks:* Memory bandwidth / latency, MPI functions, OpenMP constructs
- *NAS Parallel Benchmarks (NPB):* OpenMP, MPI, MPI+OpenMP
- *Applications:* OVERFLOW, Cart3D, WRF
- Results reported without extensive code modifications

# Summary Performance Results

- System stability initially an issue but situation improved as MPSS (Many-core Platform Software Stack) has matured
- Running codes in Native modes lead to wasted resources
- MPI and OpenMP overhead very high on Phi compared to on host
- Off-load mode has significant overhead associated with data transfer
- Optimal load balancing in Symmetric mode is extremely challenging
- Hybrid code in Symmetric mode yields best performance due to reduced MPI communication and improved resource utilization
- Obtaining good performance on Phi is not simple – requires careful design of data structure and memory layout, and lots of parallelism
- Phi not ready for prime time, but next generation looks promising due to no host and several other architectural improvements

- Extensive details in SC2013 paper by S. Saini et al.: *"An early performance evaluation of many integrated core architecture based SGI rackable computing system"*

# Big Data

NASA has enormous collections of observational and model data

- <u>Observational Data</u>
  - Tens of satellites and telescopes producing multi-petabytes of data per year
  - SMD's Earth Science Division operates 12 DAACs (archive centers) containing ~10 PB of data
  - Solar Dynamics Observatory (SDO) satellite produces 1 GB per minute; translates to ~3 PB over its 5-year life cycle


- <u>Model / Simulation Data</u>
  - NAS Division has 20 PB of unique data in global filesystems and 115 PB of archive storage
  - MITgcm code running at 1/48th degree resolution on 35K cores produced 1.4 PB during its 5-day run; full simulation will produce 9–18 PB

DISE (Data Intensive Supercomputing Environment) integrates Big Data and Big Compute to support analysis and analytics of NASA data

*Fun Fact:* The term "Big Data" was first used by Michael Cox & David Ellsworth of NAS Division in a Visualization '97 paper: *"Visualizing flow around an airframe"*, where largest dataset considered was 7.5 GB

# Big Data Challenges for Users

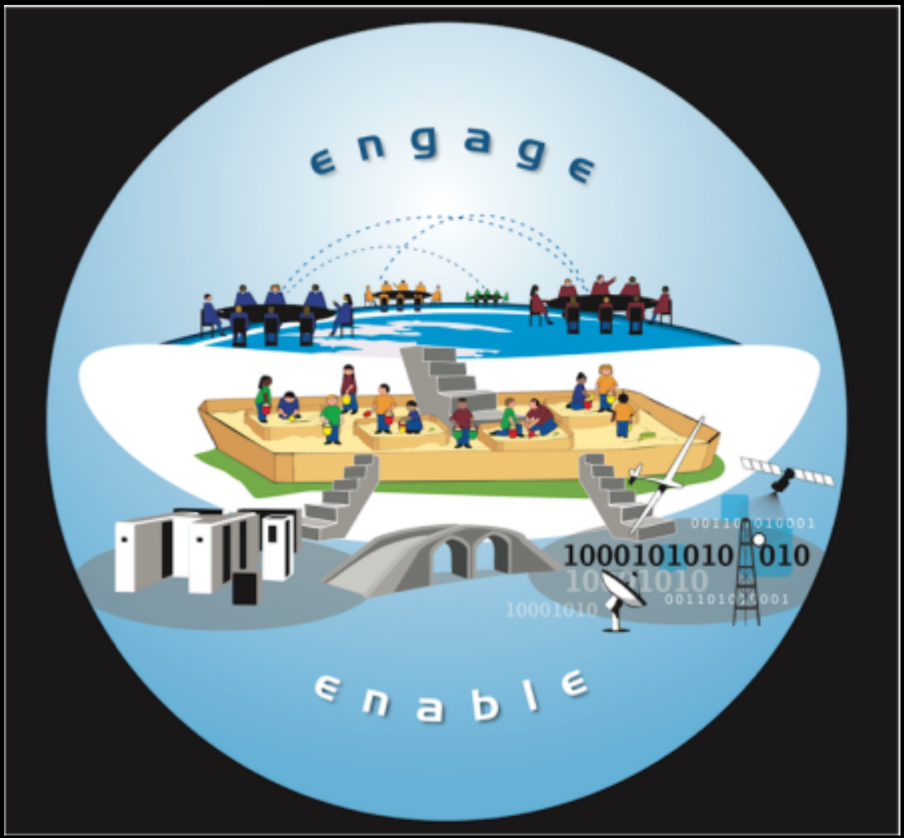
Conducted survey of NASA projects dealing with Big Data to gather user requirements


Developing a roadmap including prototype implementations

- ***Data Discovery:*** Finding what data is available and where
- ***Data Management:*** Transferring very large datasets from archives to computational resources
- ***Tools / Models / Algorithms:*** Developing analysis & analytics software at scale
- ***Analysis Workflow:*** Handling increasingly complex processing pipelines
- ***Analysis / Analytics Infrastructure:*** Dealing with inadequacy of available heterogeneous resources
- ***Collaboration Environments:*** Difficulty with sharing knowledge across a wider community

# NASA Earth Exchange (NEX)

A collaborative environment that brings scientists and researchers together in a knowledge-based social network along with observational data, tools, and computing power to provide transparency and accelerate research




**VISION**

To provide "*Science as a Service*" to the Earth science community addressing global environmental challenges

**GOAL**

To improve efficiency and expand the scope of NASA Earth science technology, research, and applications programs

# NEX Environment


**Collaboration Portal (over 400 members)**

Tools, Models, Workflows, Papers, Data

**Compute Resources (over 3 PF computing)**

Sandbox for experimentation, HPC (Pleiades)


**Data Repository (over 1.3 PB of data)**

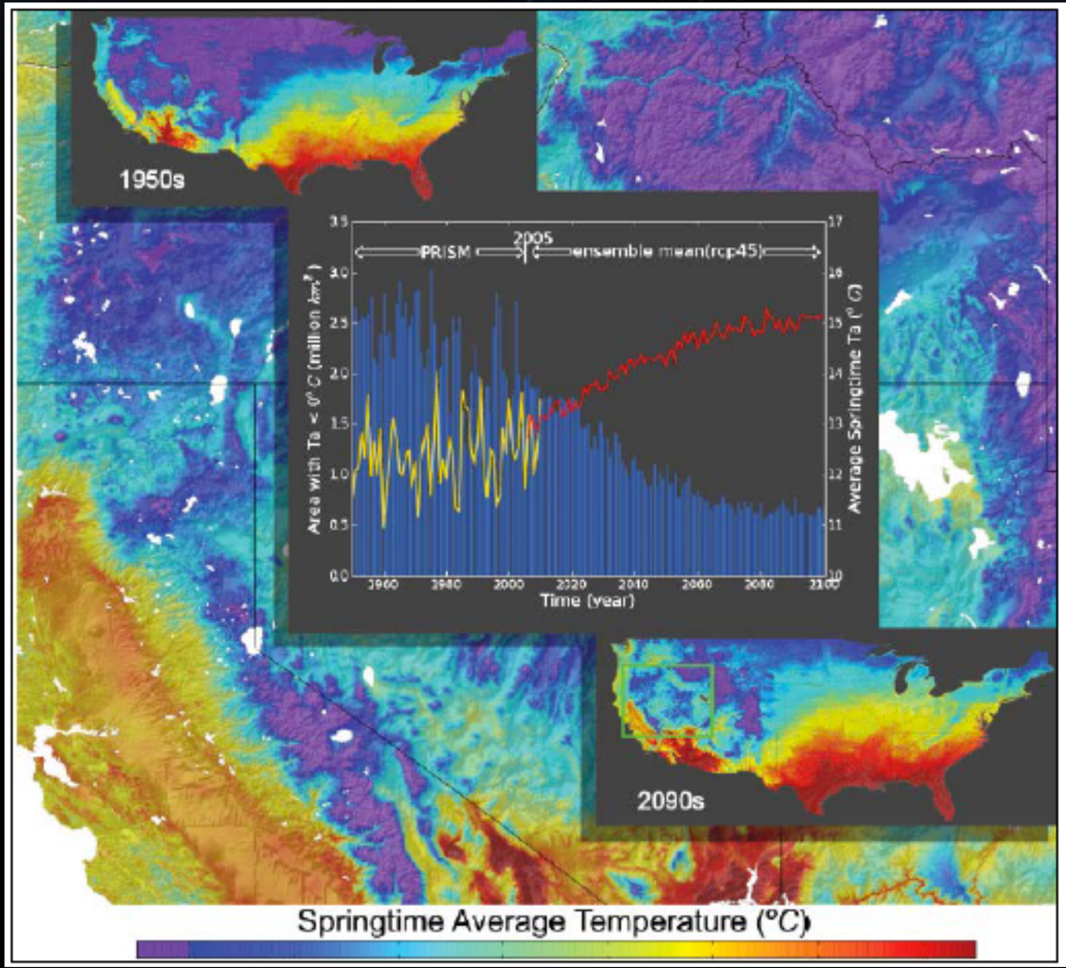
Working copies of Observational and Project data

- Collaboration portal open to all Earth scientists
- Sandbox currently available to a subset of scientists with NASA credentials
- HPC resources available only to approved projects with allocation
- OpenNEX, a collaboration with Amazon, provides NEX datasets to the wider Earth science community

# High-Resolution Climate Projections

## National Climate Assessment

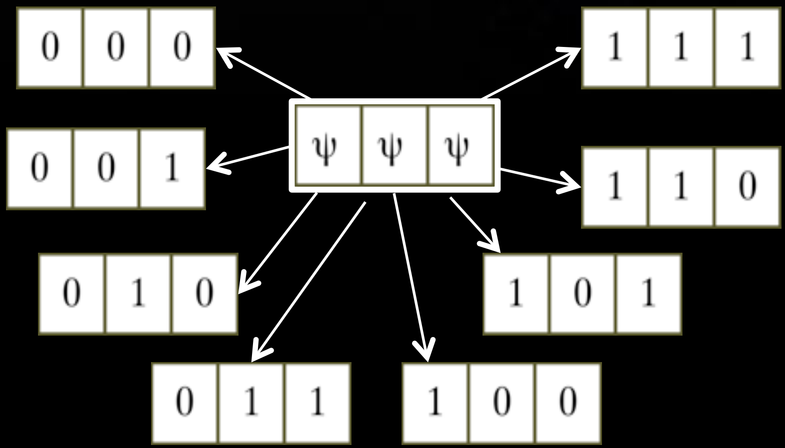
- Statistical downscaling of coarse data from CMIP5 (for IPCC) for conterminous U.S. to obtain high-resolution predictions at local scale
- ~800m grid resolution
- Spring (March–May), 1950–2099
- Mean temperature projected to increase from 12°C to 15°C assuming greenhouse gas emissions stabilize in 2050
- Area at or below 0°C isotherm decreases from 2.5M sq. km to 0.6 sq. km

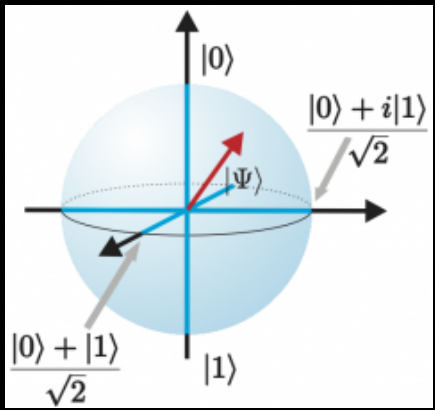



- Details in paper by B. Thrasher et al.: *"Downscaled climate projections suitable for resource management,"* Eos, Vol. 94, No. 37, Sept. 2013, pp. 321-323

# Quantum Computing

- Quantum mechanics deals with physical phenomena at very small scales (~100 nm) or at very low temperatures (few K) where actions are quantized
- The outcome of a quantum experiment is probabilistically associated both with what was done before the measurement and how the measurement was conducted
- Qubits (quantum bits) can exist in a superposition of states, allowing *n* qubits to represent $2^n$ states simultaneously
- At the end of a computation, on measurement, the system collapses into a classical state returning only one bit string as a possible solution

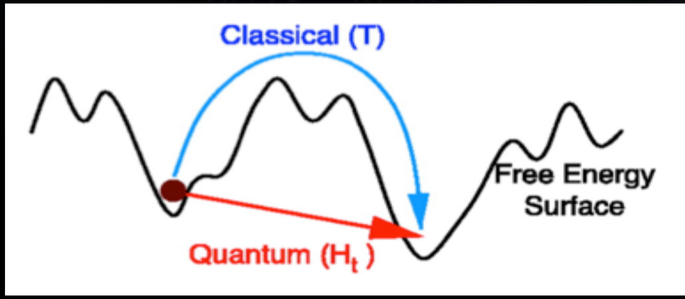


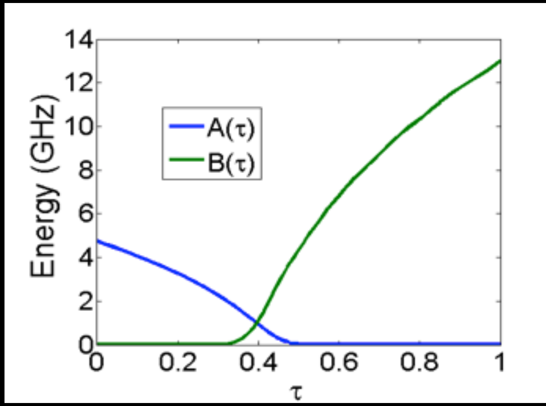
# Quantum Annealing

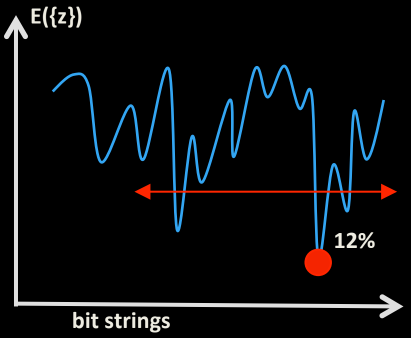
A physical technique to solve combinatorial optimization problems in QUBO (Quadratic Unconstrained Binary Optimization)

$$E(z_1, z_2, \dots z_n) = \underbrace{\left(1 - \frac{t}{T}\right)}_{A(t)} H_O(\{z\}) + \underbrace{\frac{t}{T}}_{B(t)} H_P(\{z\})$$

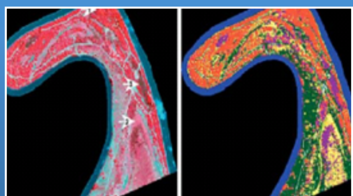



- *N*-bit string of unknown variables {*z*}
- $H_0$: Hamiltonian with known ground state
- $H_P$: Hamiltonian whose ground state represents the solution to the problem
- *A(t)* is slowly (adiabatically) lowered to zero while maintaining minimum energy of the system at all times
- Solution is the configuration {*z*} that produces the minimum *E* with a non-zero probability



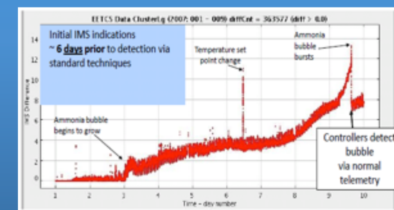



# NASA and Quantum Computing

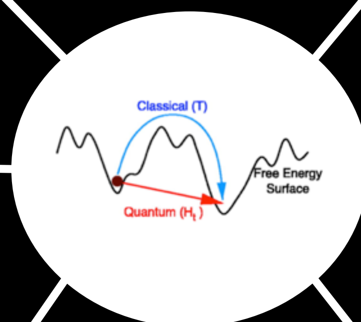


Data Analysis and Data Fusion

Anomaly Detection and Decision Making

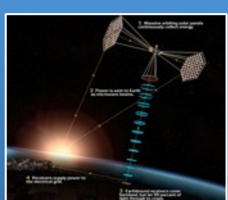



Air Traffic Management




V&V and optimal sensor placement

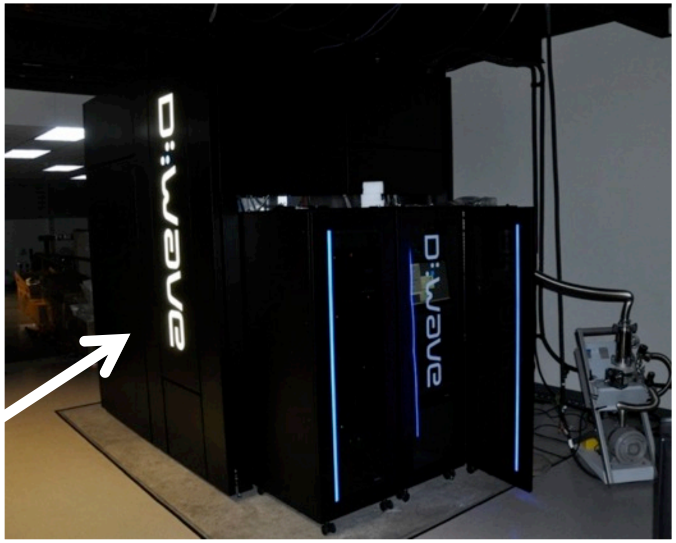
Mission Planning and Scheduling, and Coordination

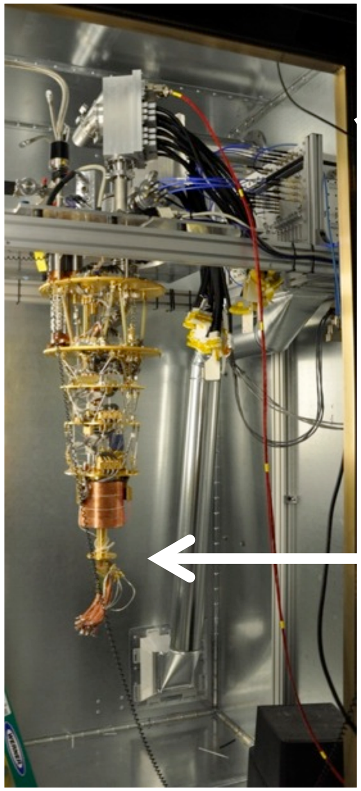


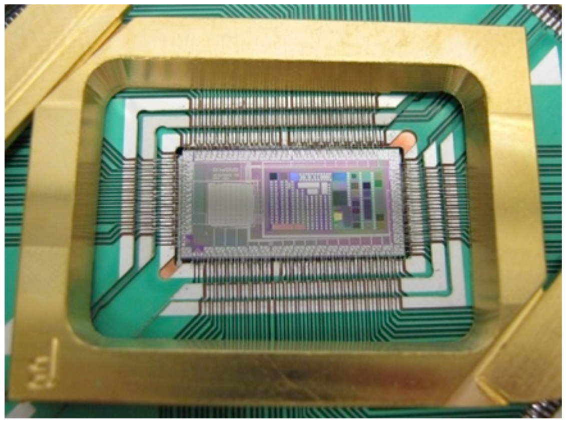
Topologically aware Parallel Computing

# D-Wave Two System

- Collaboration among NASA, Google, and USRA led to installation of system at NAS Division
- 512-qubit Vesuvius processor (to be continuously upgraded over the next 4+ years)
- 10 kg of metal in vacuum at 15 mK
- Magnetic shielding to 1 nanoTesla
- Protected from transient vibrations
- Single run takes 20 μsecs
- Uses 12 kW of electrical power



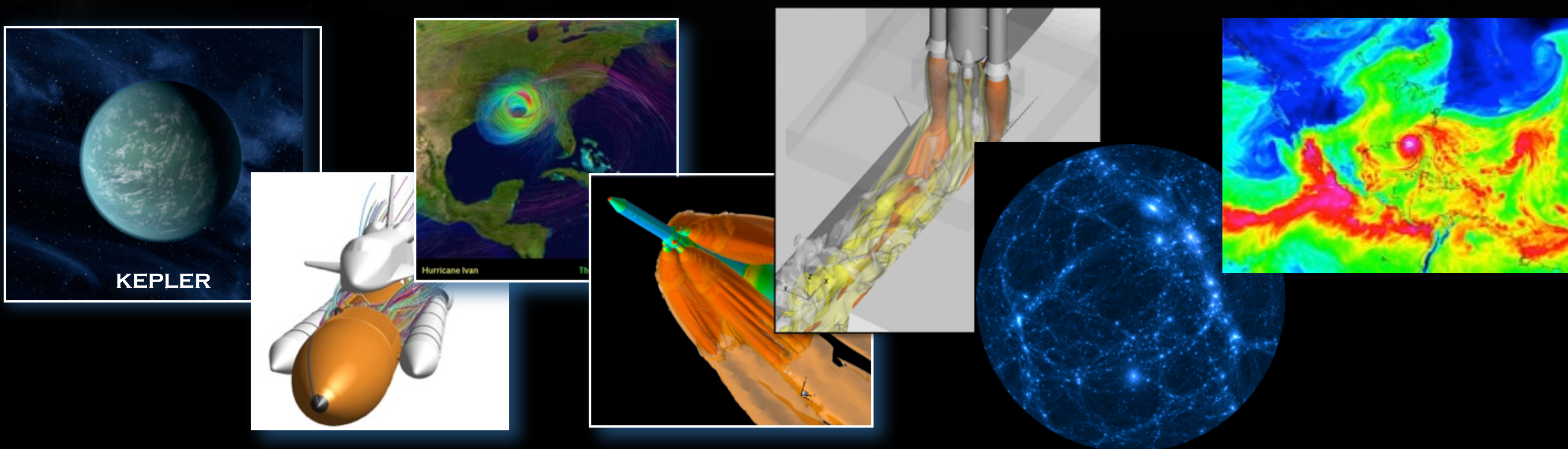





Focused on solving discrete optimization problems using quantum annealing

# NAS Focus

*Enable the science & engineering required to meet NASA's missions and goals*




*Effective, stable, production-level HPC environment*

*Advanced technologies to meet future goals*

# Thank You!

## Questions?

rupak.biswas@nasa.gov