NASA Advanced Computing Environment for Science & Engineering

Dr. Rupak Biswas

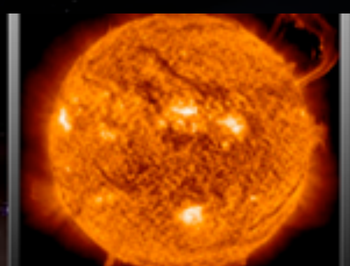
Director, Exploration Technology Directorate
Manager, High End Computing Capability (HECC) Project

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

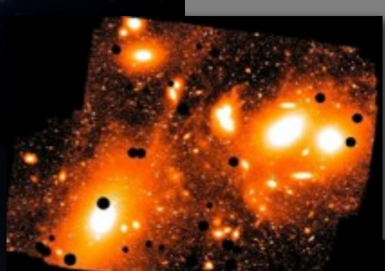
Argonne Training Program on Extreme-Scale Computing (ATPESC)
Q Center, St. Charles, IL, 3 August 2017

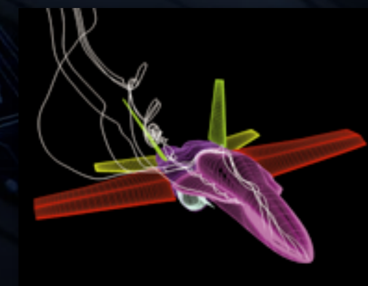
NASA Overview: Mission Directorates

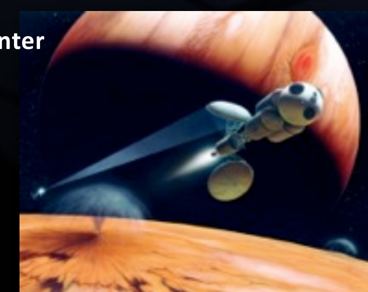
- **Vision**: *To reach for new heights and reveal the unknown so that what we do and learn will benefit all humankind*
- **Mission**: *To pioneer the future in space exploration, scientific discovery, and aeronautics research*
- **Aeronautics Research (ARMD):** Pioneer and prove new flight technologies 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



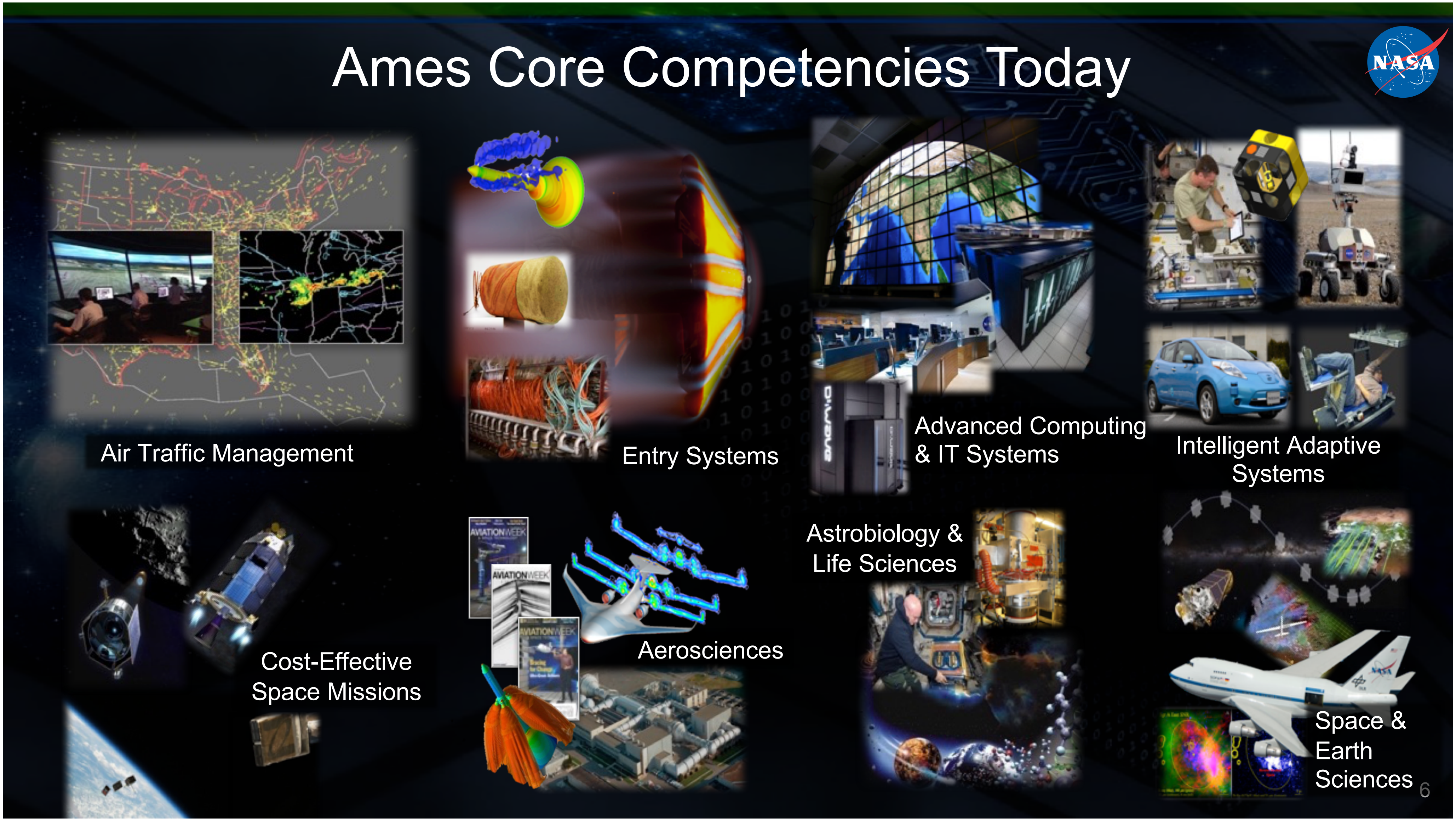




Current NASA Focus Areas

NASA Ames Research Center

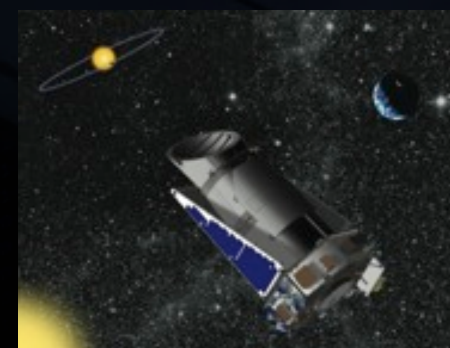
- **Occupants**: ~1,130 civil servants; ~2,100 contractors; ~1,650 tenants; 855 summer students (in 2016)
- **FY2016 Budget**: ~$915M (including reimbursable and Enhanced Use Lease (EUL) revenue)
- **Real Estate**: ~1,900 acres (400 acres security perimeter); 5M building ft^2; Airfield: ~9,000 and 8,000 ft runways


Ames Core Competencies Today
NASA
Air Traffic Management
Entry Systems
Advanced Computing & IT Systems
Intelligent Adaptive Systems
Cost-Effective Space Missions
AVIATION WEEK
Aerosciences
Astrobiology & Life Sciences
Space & Earth Sciences
6

Need for Advanced Computing

Enables modeling, simulation, analysis, and decision-making

- Digital experiments and physical experiments are tradable
- Physical systems and live tests 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

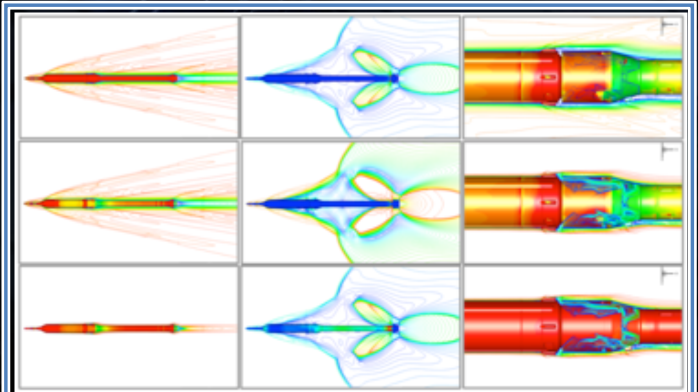


- Decades of exponentially advancing computing technology has enabled dramatic improvements in cost, speed, and accuracy – in addition to providing a predictive capability
- Many problems pose extremely difficult combinatorial optimization challenges that can only be solved accurately using advanced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

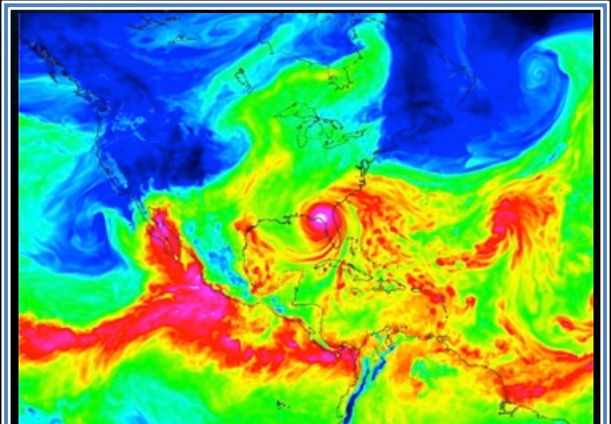
Advanced Computing Environment

NASA's Diverse HPC Requirements

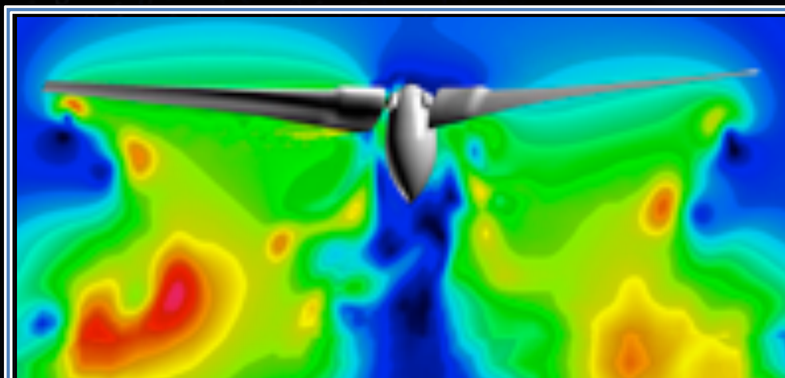
- Engineering requires HPC resources that can process large ensembles of moderate-scale computations to efficiently explore design space ***(high throughput / capacity)***
- Research requires HPC resources that can handle high-fidelity long-running large-scale computations to advance theoretical understanding ***(leadership / capability)***
- Time-sensitive mission-critical applications require HPC resources on demand ***(high availability / maintain readiness)***



Aerodynamic database generation



Real-time hurricane prediction

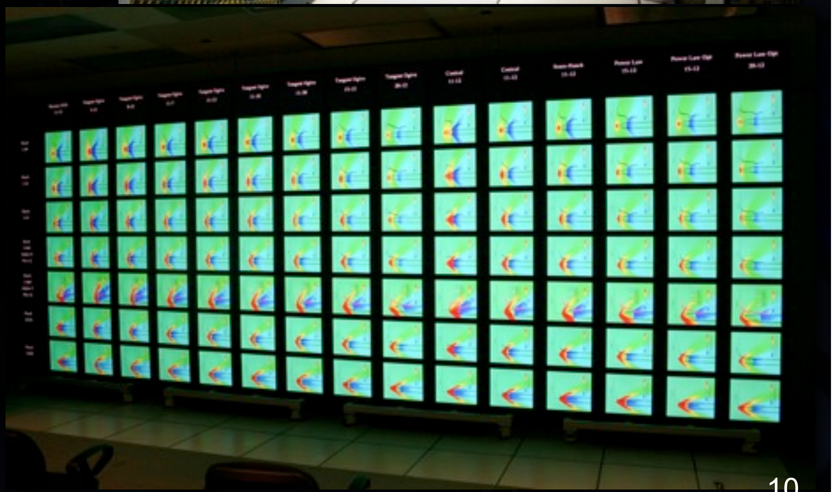


Rotary wing unsteady aerodynamics

Balanced HPC Environment

Computing Systems

- ***Pleiades:*** 246K-core SGI Altix ICE (now HPE) with 4 generations of Intel Xeon (64 nodes GPU-enhanced: Nvidia M2090, K40; 32 nodes have Phi 5110P); 938 TB RAM; 7.25 PF peak (#15 on TOP500, #10 on HPCG)
- ***Electra:*** 32K-core Altix ICE with Intel Broadwell; modular container; 147 TB RAM; 1.24 PF peak
- ***Merope:*** 22K-core Altix ICE with Intel Westmere; 86 TB RAM; 252 TF peak
- ***Endeavour:*** Two SGI UV2000 nodes with 2 and 4 TB shared memory SSI via NUMALink-6; 32 TF peak
- ***hyperwall:*** 2560-core Intel Ivy Bridge, 128-node Nvidia GeForce GTX78 cluster for large-scale rendering & concurrent visualization (240M pixels)



Data Storage

- 49 PB of RAID over 7 Lustre filesystems
- 490 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

Modular Supercomputing Facility (MSF)

Prototype MSF (FY17)

- Modular container currently holds Electra (16 Broadwell-based racks)
- External air fan cooling; switch to adiabatic evaporative cooling when needed
- PUE between 1.03 and 1.05; resulting in 93% power savings and 99.4% water use reduction over our traditional computer floor
- Current pad has 2.5 MW of electrical power and can accommodate 2 modules
- In production use since Jan ‘17
- Second module to be added in Oct ’17, bringing Electra to 4.78 PF peak

Full MSF (FY18 – FY22)

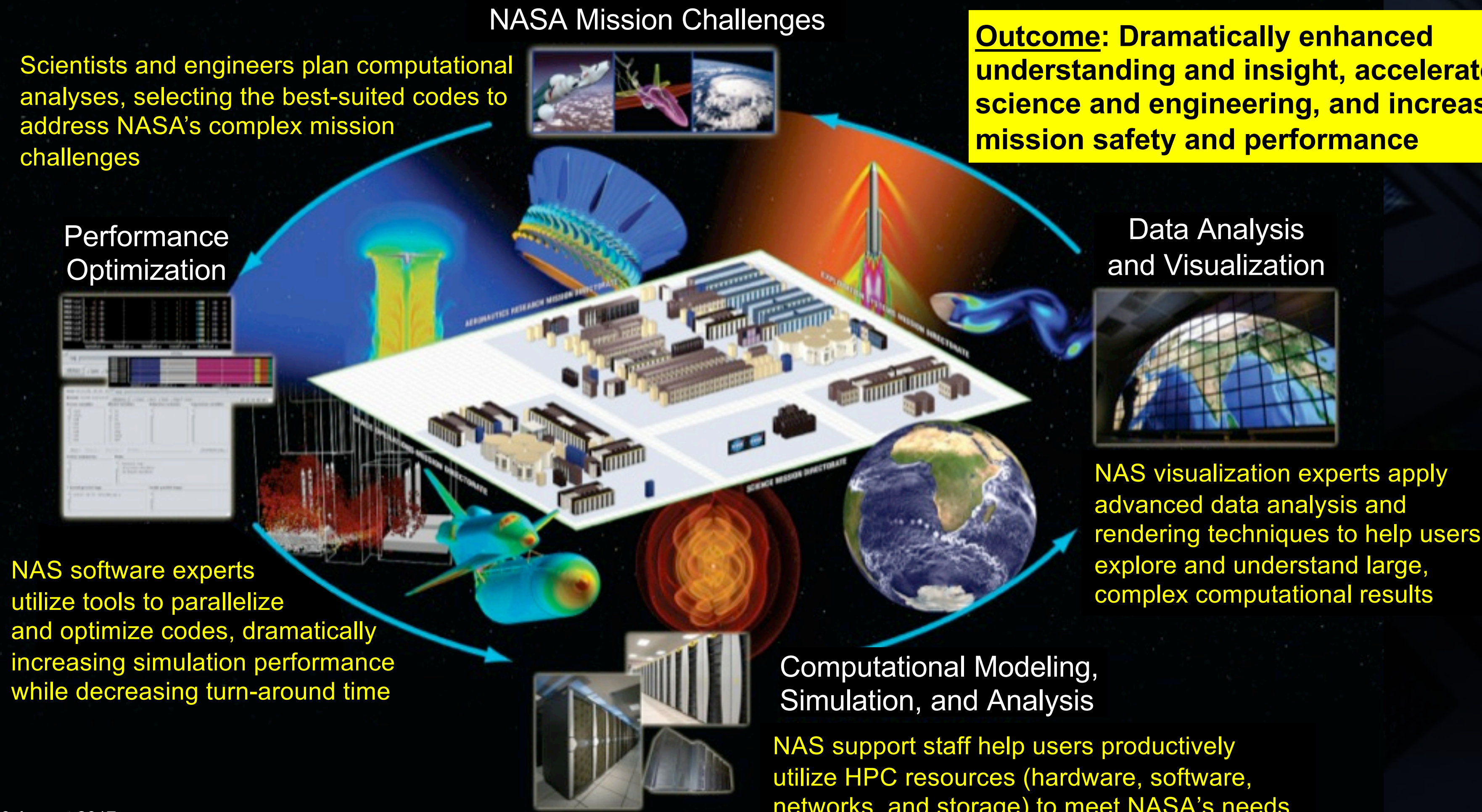
- Larger second pad with 15 MW electrical power and associated switchgear
- Ability to hold up to 16 modular units
- Flexibility to rapidly modify and react to changes in NASA requirements, computing technology, and facility innovations

Prototype MSF hosting Electra

Artist’s rendering of future MSF

Integrated Spiral Support Services

<u>Outcome</u>: Dramatically enhanced understanding and insight, accelerated science and engineering, and increased mission safety and performance



NASA Earth Exchange (NEX)

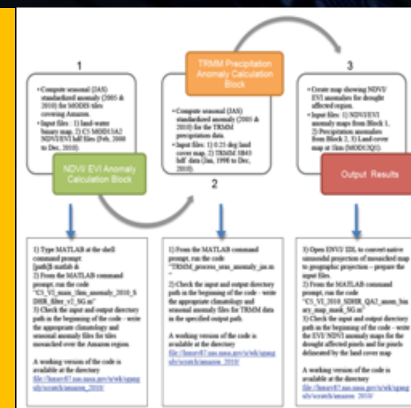
A virtual collaborative environment that brings scientists and researchers together in a knowledge-based social network along with observational data, necessary tools, and computing power to provide transparency and accelerate innovation: **Science-as-a-Service**

VIRTUAL COLLABORATION

Over 650 members

CENTRALIZED DATA REPOSITORY

Over 3.5 PB of observational data



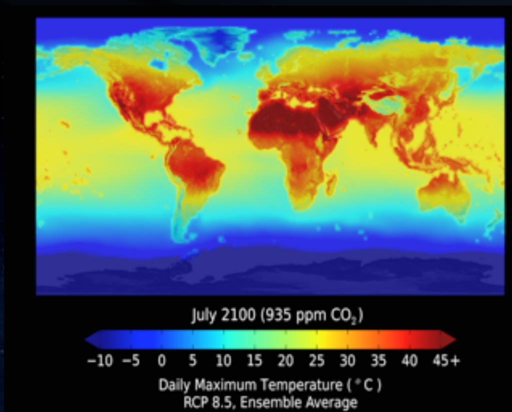
SCALABLE COMPUTING

Heterogeneous and remote, secure access

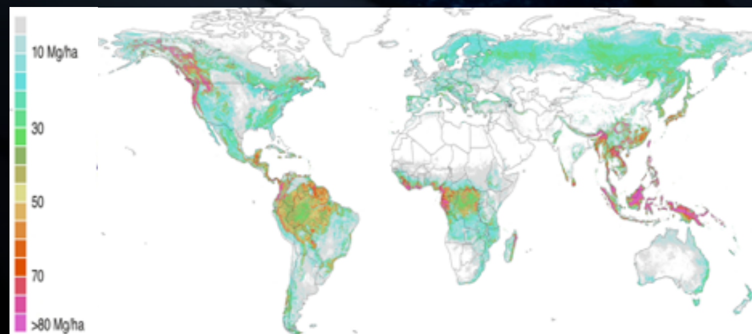
KNOWLEDGE

Workflows, virtual machine images, model codes, and reusable software

Science via NEX



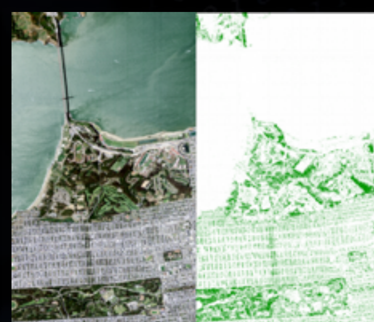
High-resolution projections for climate impact studies

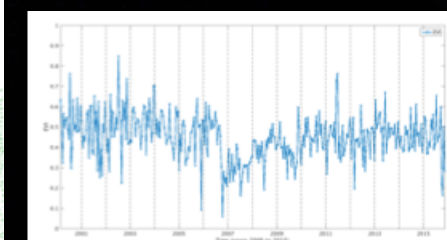


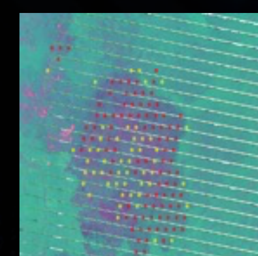
Global vegetation biomass at 100m resolution by blending data from 4 different satellites

High-resolution monthly global data for monitoring crops, forests, and water resources

Sample publication using NEX environment:
Nature 532.7599 (2016): 357



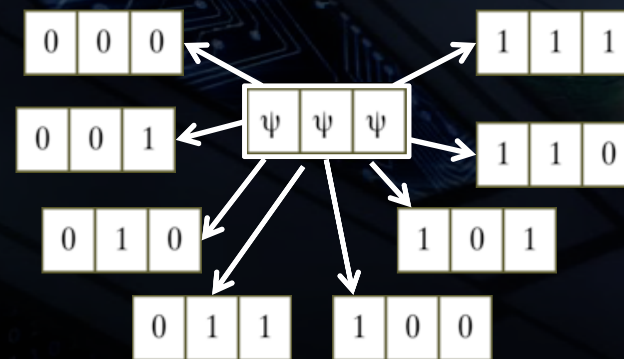




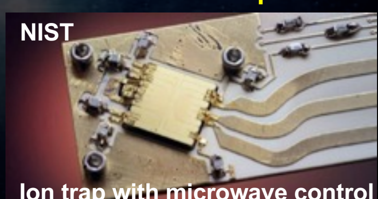
Machine learning and data mining – moving toward data-driven approaches

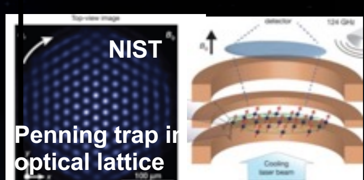
Quantum Computing 101

- Quantum mechanics deals with physical phenomena at very small scales (~100nm) and 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 to a classical state and returns only one bit string as a possible solution

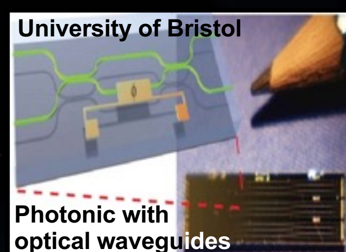


Numerous Implementations

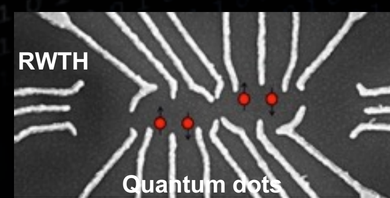


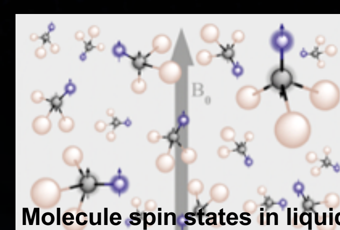


Trapped Ions and Neutral Atoms

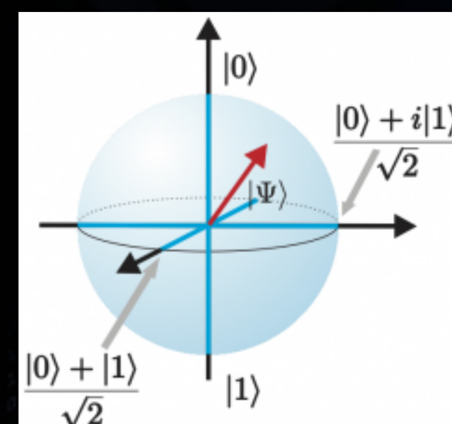


Photonic Quantum Chips



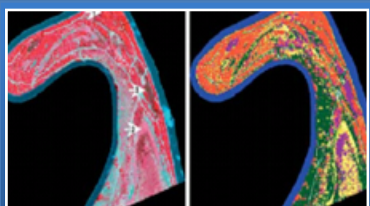


Nanoelectronics, NMR, Diamond Chips, etc.

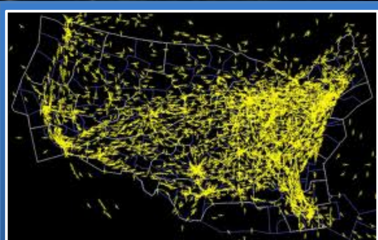


Quantum Computing for NASA Applications

Objective: Find "better" solution
- Faster
- More precise
- Not found by classical algorithm

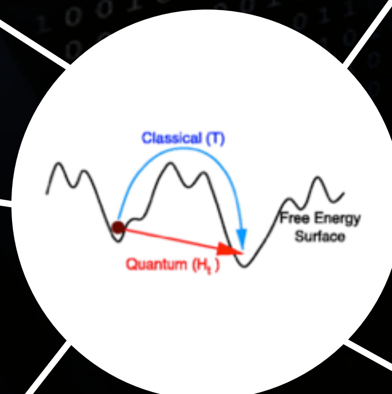


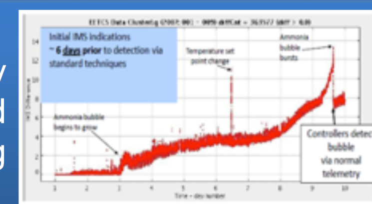
Data Analysis and Data Fusion



Air Traffic Management

Mission Planning, Scheduling, and Coordination





Anomaly Detection and Decision Making

V&V and Optimal Sensor Placement

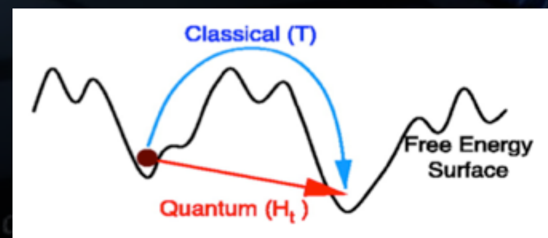
Topologically-aware Parallel Computing

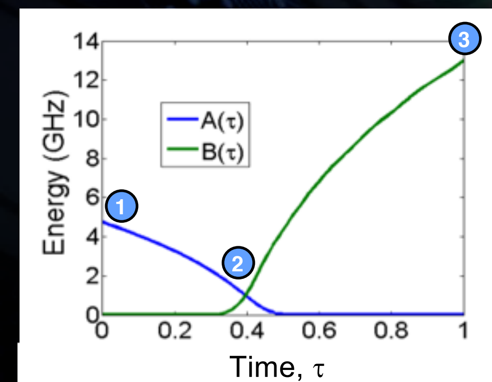
Common Feature: Intractable (NP-hard / NP-complete) problems!

Quantum Annealing

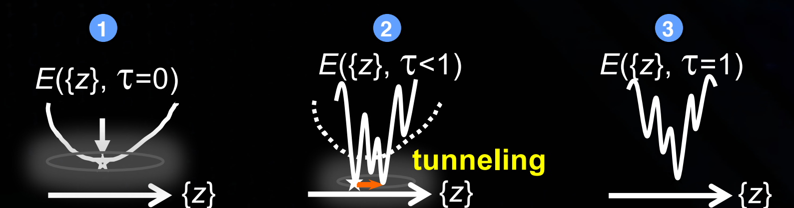
A physical technique to solve combinatorial optimization problems

$$E(z_1, z_2, \dots z_n) = \underbrace{\left(1 - \frac{t}{T}\right)}_{A(t)} H_0(\{z\}) + \underbrace{\frac{t}{T}}_{B(t)} H_P(\{z\})$$





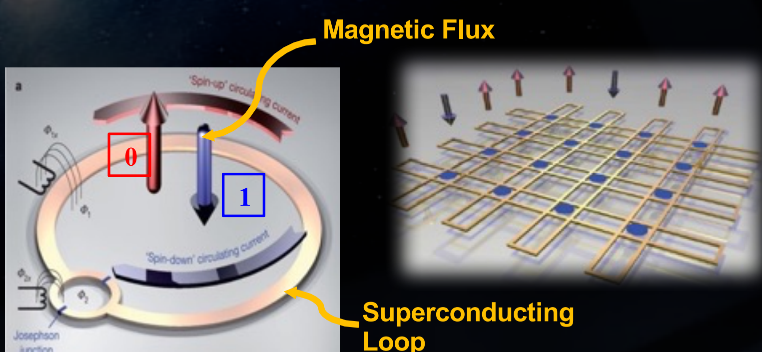
- *N*-bit string of unknown variables {*z*}
- H_0: Hamiltonian with known ground state
- H_P: Hamiltonian whose ground state represents solution to the problem
- Large *A(t)* responsible for quantum fluctuations slowly (adiabatically) lowered to zero while maintaining minimum energy of the system at all times
- In conjunction, cost function of interest *B(t)* gradually turned on
- Transitions between states occur via tunneling through barriers due to quantum fluctuations
- Solution is configuration {*z*} that produces minimum *E* with non-zero probability
- Method similar to simulated annealing where transitions between states occur via jumping over barriers due to thermal fluctuations

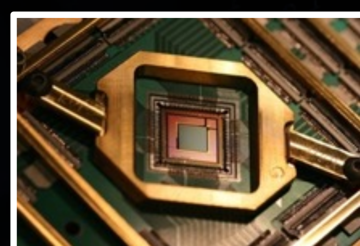


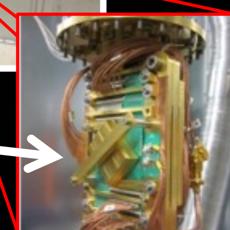
1. *Initialize in an easy-to-prepare full quantum superposition*
2. *Quantum states explored by quantum tunneling*
3. *Final state a bit-string encoding solution with probability*

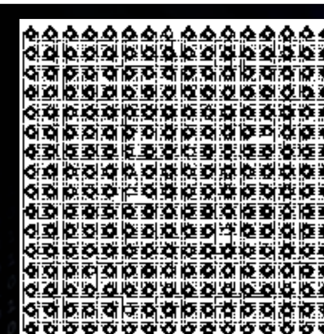
D-Wave System Hardware

- Collaboration with Google and USRA via Space Act Agreement led to installation of system at NASA Ames in early 2013
- Started with 512-qubit Vesuvius processor – currently 2031-bit Whistler
- 10 kg of metal in vacuum at ~15 mK
- Magnetic shielding to 1 nanoTesla
- Protected from transient vibrations
- Single annealing typically 20 μs
- Typical run of 10K anneals (incl. reset & readout takes ~4 sec)
- Uses 15 kW of electrical power









Focus on solving discrete optimization problems using quantum annealing

Programming the D-Wave System

1 Map the target combinatorial optimization problem into QUBO

No general algorithms but smart mathematical tricks (penalty functions, locality reduction, etc.)

$$\alpha_{ijk} z_i z_j z_k$$

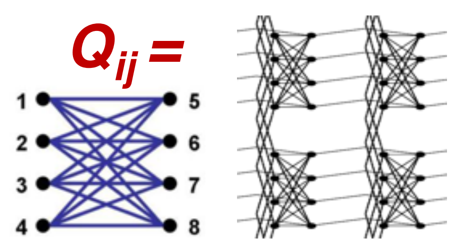
$$\alpha_{ijk}\ y_{ij} z_k + \beta_{ijk}(3y_{ij} - 2z_i y_{ij} - 2z_j y_{ij} + z_i z_j)$$

$$\sum_{ij} Q_{ij} z_i z_j \rightarrow \sum_i h_i s_i + \sum_{i,j} J_{ij} s_i s_j$$

Mapping not needed for random spin-glass models

2 Embed the QUBO coupling matrix in the hardware graph of interacting qubits

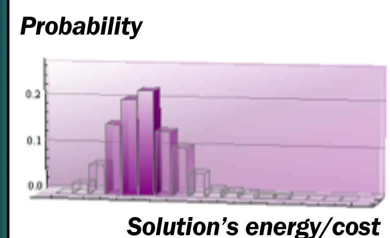
D-Wave qubit hardware connectivity is a Chimera graph, so embedding methods mostly based on heuristics



Embedding not needed for native Chimera problems

3 Run the problem several times and collect statistics

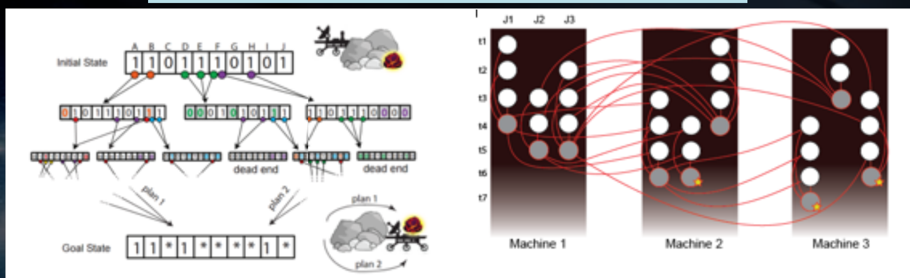
Use symmetries, permutations, and error correction to eliminate the systemic hardware errors and check the solutions



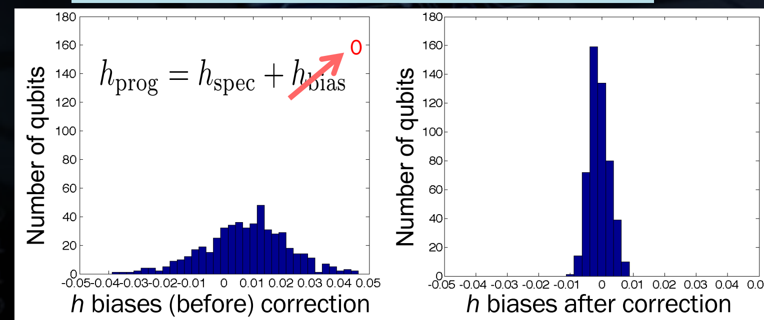
Performance can be improved dramatically with smart pre-/post-processing

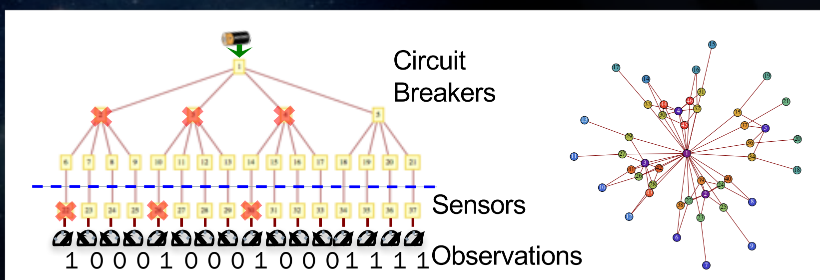
Current NASA Research in Quantum

Complex Planning and Scheduling



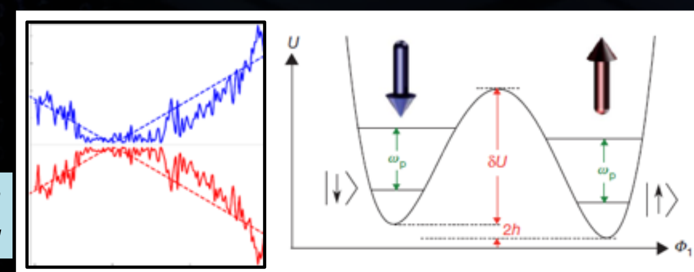
Calibration of Quantum Annealers

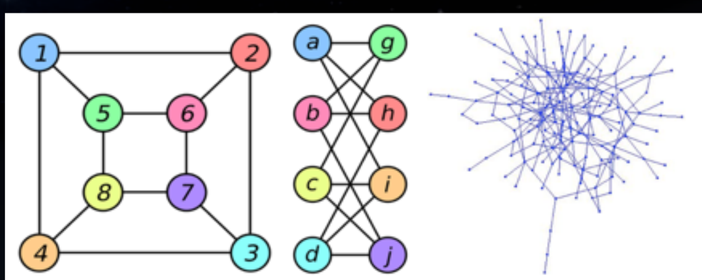




Graph-based Fault Detection

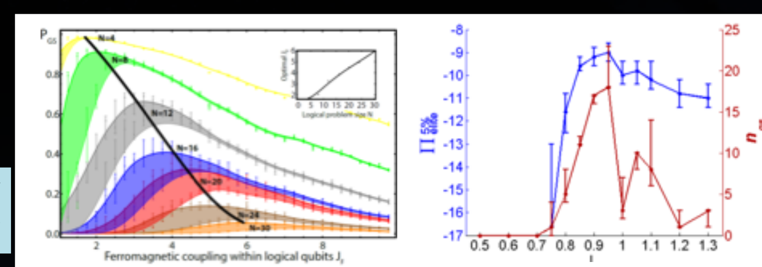
Effect of Noise on Quantum Annealing





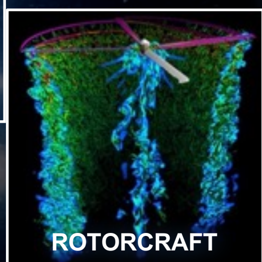
Graph Isomorphism

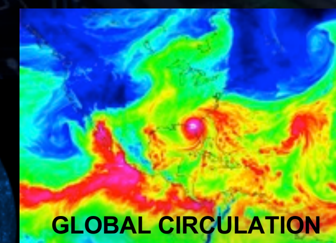
Optimal Embedding and Parameter Setting



Advanced Computing Mission

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





Effective, stable, production-level HPC environment

Advanced technologies to meet future goals