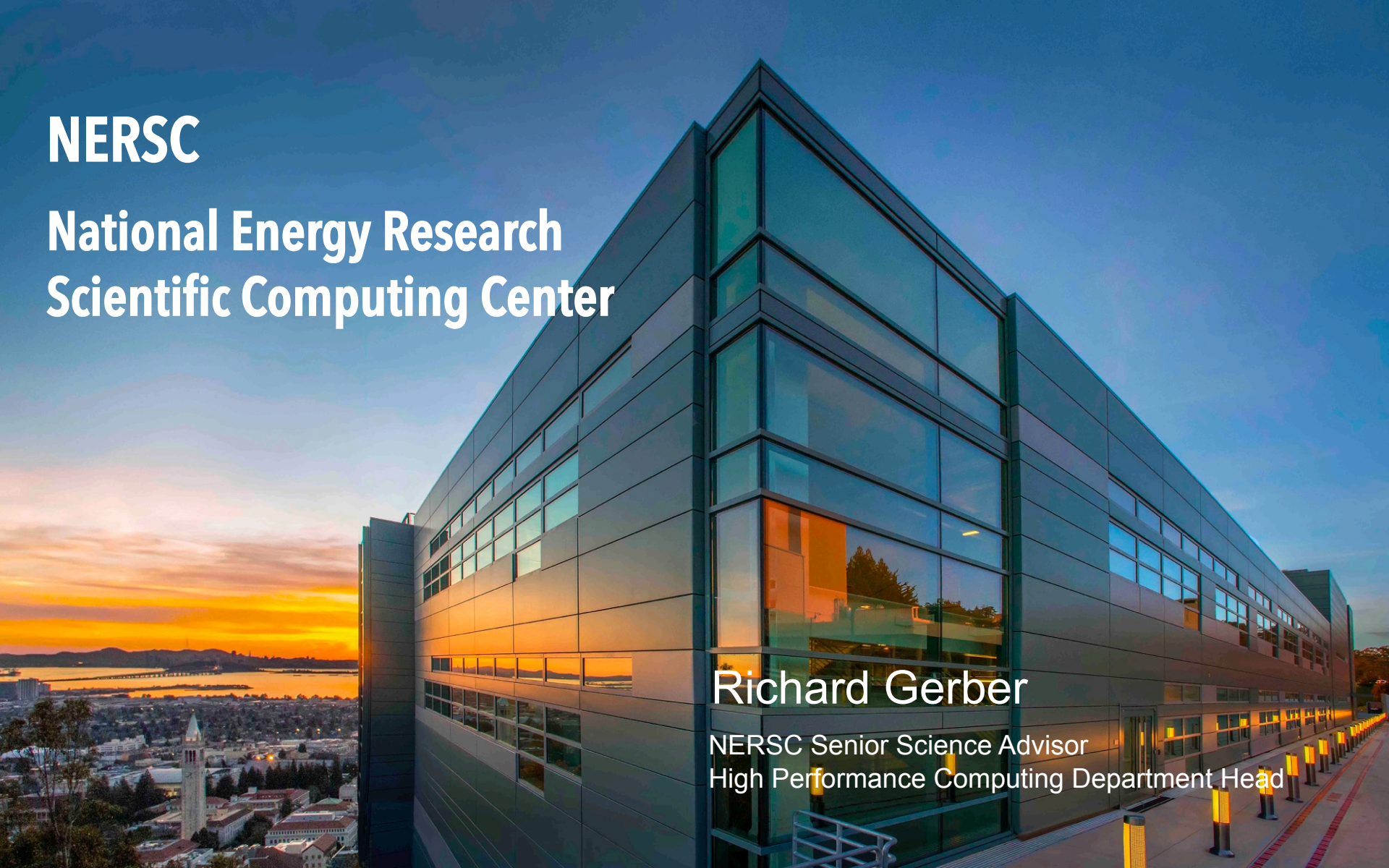


NERSC

National Energy Research Scientific Computing Center

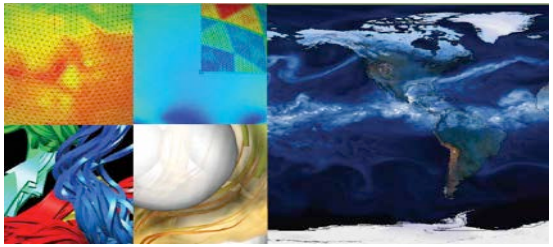
Richard Gerber

NERSC Senior Science Advisor
High Performance Computing Department Head

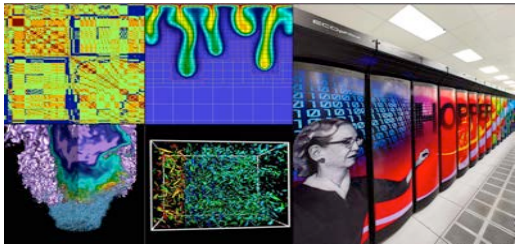
NERSC: the Mission HPC Facility for DOE Office of Science Research

U.S. DEPARTMENT OF ENERGY | Office of Science

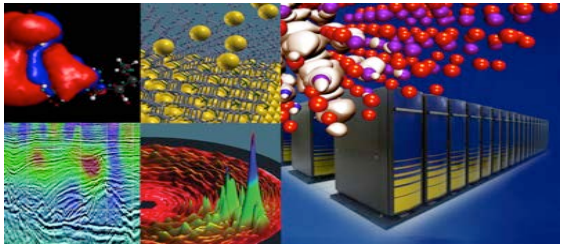
Largest funder of physical science research in the U.S.



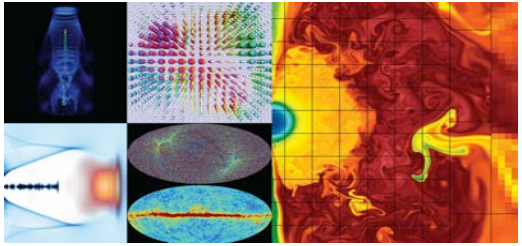
Bio Energy, Environment



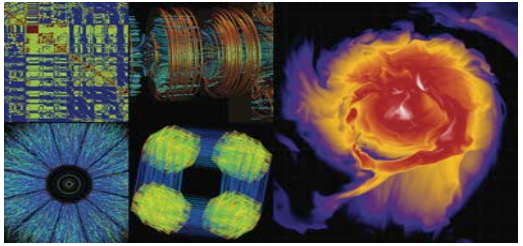
Computing



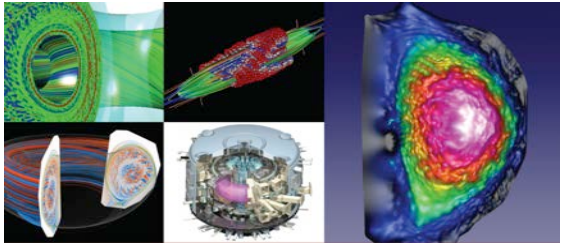
Materials, Chemistry, Geophysics



Particle Physics, Astrophysics



Nuclear Physics



Fusion Energy, Plasma Physics

6,000 users, 700 projects, 700 codes, 48 states, 40 countries, universities & national labs

Focus on Science

NERSC supports the broad mission needs of the six DOE Office of Science program offices

7,000 users and 850 projects

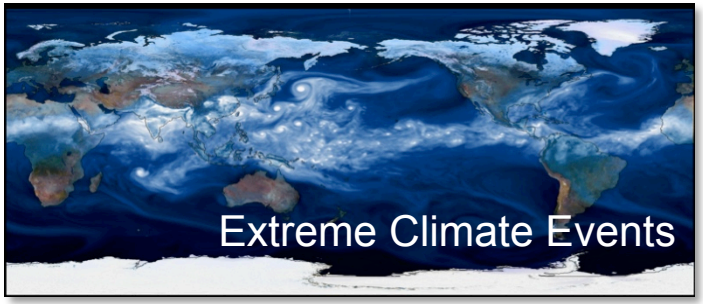
Supercomputing and data users

NERSC science engagement team provides outreach and POCs

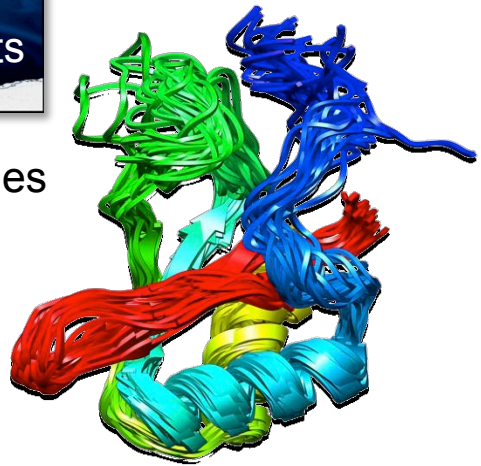
2,000 refereed publications per year

High Performance Computing is …

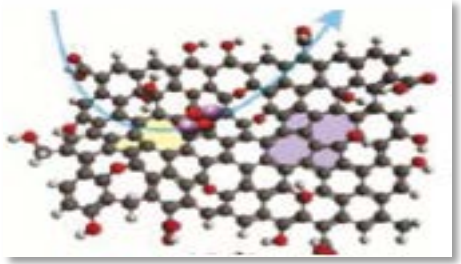
… the application of "supercomputers" to scientific computational problems that are too large for standard computers, would take them too long, would be too dangerous, or probe inaccessible realms.



Understanding How Proteins Work



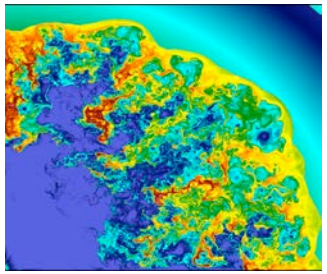
Designing Better Batteries



Science Highlights June 2017

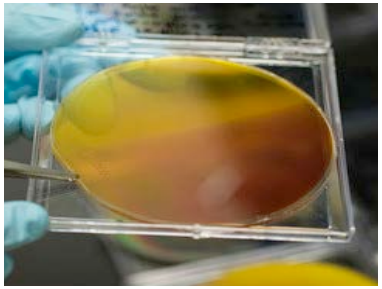
Astrophysics

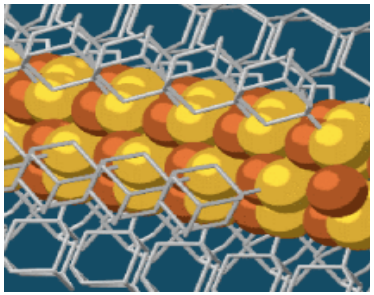
First 2D models of rare superluminous supernova reveal insight into their origin.
NERSC PI: Woosley, UC Santa Cruz.
Astrophysical Journal



Materials Science

Researchers develop a process that promises to speed the discovery of commercially viable materials to produce solar fuels. **PI: Neaton, Berkeley Lab.**
Proc. Nat. Acad. Sci.





Materials Science

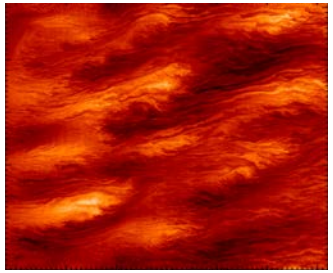
Scientists have discovered a way to use diamondoids to make electrical wires just 3 atoms wide. **NERSC PI: Devereaux, Stanford, *Nature Materials***

Atmospheric Science

3D models lead to an improved statistical representation of clouds.
NERSC PI: Ovchinnikov, Pacific NW Labs, *J. of Geophys. Rsrch: Atmospheres*

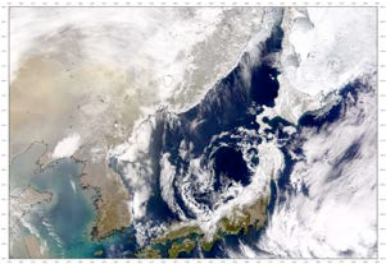
Fusion Energy

Researchers find multiscale electron energy transport in tokamak fusion reactors.
NERSC PI: Holland, UC San Diego.
Nuclear Fusion



Environment

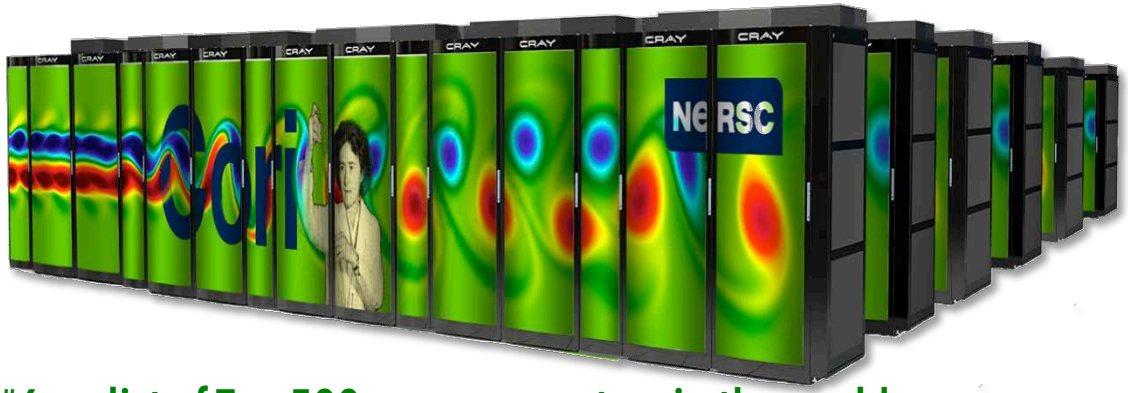
Simulations reveal that less dust leads to worse air pollution in China. **NERSC PI: Ghan, Pacific NW Labs.** ***Nature Communications***



Production High Performance Computing Systems

Cori

9,600 Intel Xeon Phi "KNL" manycore nodes
2,000 Intel Xeon "Haswell" nodes
700,000 processor cores, 1.2 PB memory
Cray XC40 / Aries Dragonfly interconnect
30 PB Lustre Cray Sonexion scratch FS
1.5 PB Burst Buffer

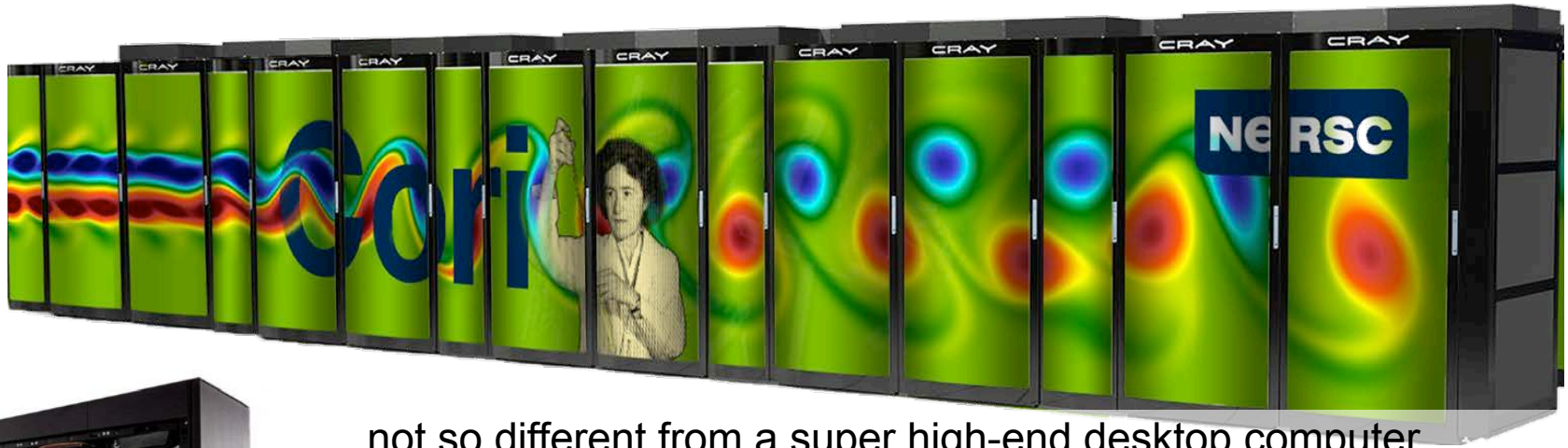


#6 on list of Top 500 supercomputers in the world

Edison

5,560 Ivy Bridge Nodes / 24 cores/node
133 K cores, 64 GB memory/node
Cray XC30 / Aries Dragonfly interconnect
6 PB Lustre Cray Sonexion scratch FS

A Supercomputer is …



… not so different from a super high-end desktop computer.

Or rather, a lot of super high-end desktop computers.

Cori has 11,000 “nodes” (each ~a powerful high-end desktop)

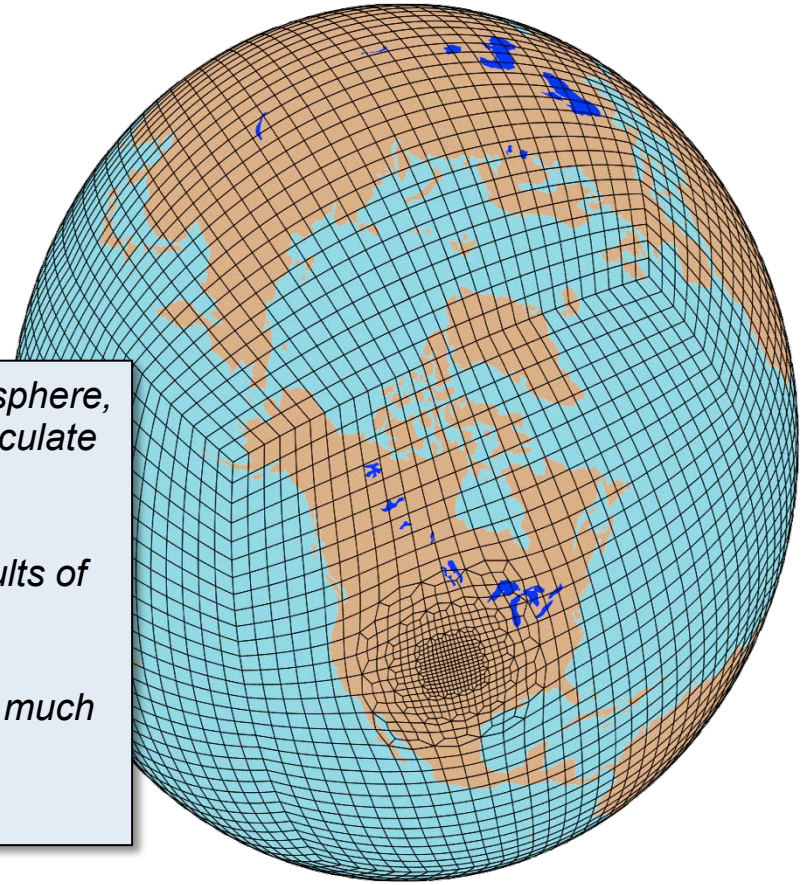
700,000 compute cores
~30x10^{15} calculations/second

7 billion people
on 4 million Earths
doing 1 calculation
each second
= 1 Cori

Parallel Computing on Supercomputers

In parallel computing, scientists divide a big task into smaller ones

"Divide and conquer"



For example, to simulate the behavior of Earth's atmosphere, you can divide it into zones and let each processor calculate what happens in each.

From time to time each processor has to send the results of its calculation to its neighbors. Without the high-speed custom network available on supercomputers, this communication step would make the calculations take much too long.

Custom Powerful Network

The nodes are all connected to each other with a high speed, low latency network.

This is what allows the nodes to "talk" to each other and ***work together to solve problems*** you could never solve on your laptop or even 150,000 laptops.

Typical point-to-point bandwidth
Supercomputer: 10 GBytes/sec
Your home: 0.02* GBytes/sec

5,000 X

Latency
Supercomputer: 1 µs
Your home computer: 20,000* µs

20,000 X

Cloud systems have slower networks

* If you're really lucky

Data

How big is 26 PBs?

338 years of HD video

½ the entire written works of mankind ever, in all languages

PBs of fast storage for files and data

Cori: 26 PB
Your laptop: 0.0005 PB
Your iPhone: 0.00005 PB

45,000 X

Write data to permanent storage

Edison: 140 GB/sec
My iMac: 0.01 GB/sec

14,000 X

Cloud systems have slower I/O and less permanent storage

HPSS tape library: 75 PB

EERE and other Energy Technologies

- ~20 NERSC projects have “EERE” in their project description.
- 100s are working on the basic science of energy technologies

  - Materials for photovoltaics, H_2O catalysis and hydrogen storage, full-spectrum & high-power LEDs, battery storage, artificial photosynthesis, biofuels, ⋯
  - Earthquake safety for nuclear power plants
  - All-liquid thermal storage materials
  - City building energy saver
  - Historical climate effects on California wind power resources
  - Understanding and Mitigating Barriers to Wind Energy Expansion in California
  - Turbulence over complex terrain: a wind-energy perspective
  - Exascale Predictive Wind Plant Flow Physics Modeling
  - Effect of offshore wind farms on storm surges
  - Nuclear waste disposal
  - CRUD formation and boron disposition on fuel rods

NERSC has users from NREL, NETL, Savannah River

SMART Mobility and Vehicle Grid Integration Analysis

Arnand Gopal & Colin Sheppard, LBNL

NERSC Director's Reserve Project 2017
1 Million NERSC Hours

- Research questions are focused on the energy impacts and efficacy of our changing transportation system through the lens of user behavior and decision-making in both the short and long run time frames.
- Along with analysis of changing modes of mobility, the project is conducting detailed work on vehicle-grid integration to analyze the potential for EVs to support the grid through management of uni-directional or bi-direction vehicle charging.
- This effort requires an analytical approach that captures the expected behaviors of EV drivers in how they choose to charge their vehicles and whether they will elect to participate in vehicle to grid exchanges or managed charging sessions.

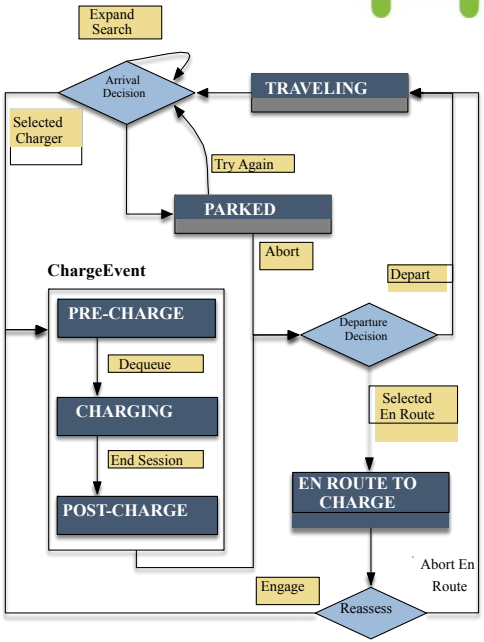


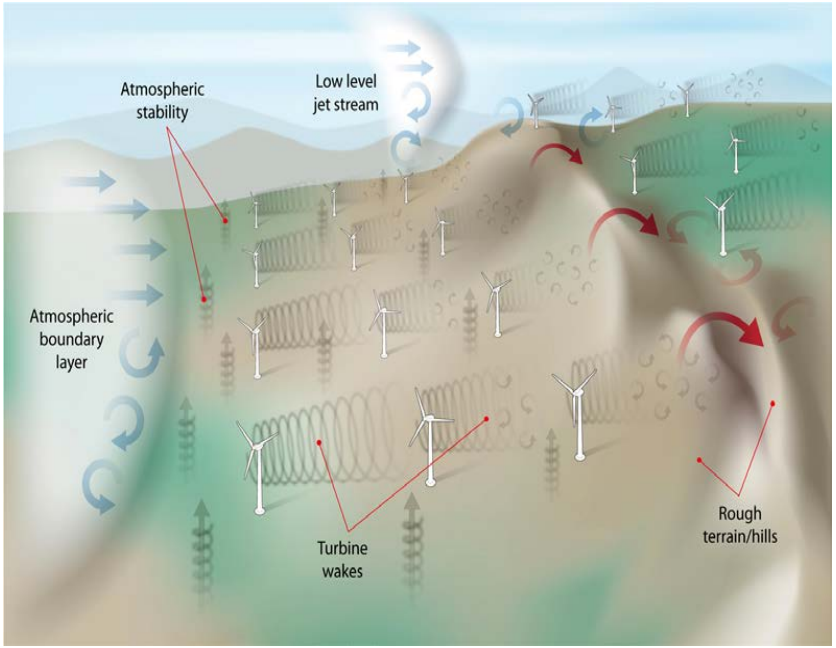
Figure 4: States (dark blue), actions (yellow), and decisions (light blue) of agents in BEAM.

Predictive Simulations of Complex Flow in Wind Farms

Matthew Barone, Stefan Domino
Sandia (NM) National Laboratories
Michael Sprague, Matthew Churchfield
National Renewable Energy Laboratory

ALCC Project 2017
10.7 Million NERSC Hours

- DOE's Wind Power Program targeting significant reductions in the cost of wind energy through its Atmosphere to Electrons (A2e) program
- DOE EERE Wind and Power Technologies Office committed to developing technologies to enable 35% of U.S. electric supply by 2050
- Aimed at improving fundamental understanding of the complex physics governing wind flow into and through wind plant.
- Accurate predictive simulations reduce uncertainty for project planning and financing.



Complex terrain can lower efficiency by 30%
Turbines in farms experience fail more often
1% improvement in performance = $100 M in U.S. savings
2% improvement saves $1B annually by 2030

NERSC at a Glance

A U.S. Department of Energy Office of Science User Facility
Provides High Performance Computing and Data Systems and Services
Unclassified Basic and Applied Research in Energy-Related Fields
6,000 users, 750 different scientific projects
Located at Lawrence Berkeley National Lab, Berkeley, CA
Permanent Staff of about 70