

What's so super about supercomputers?



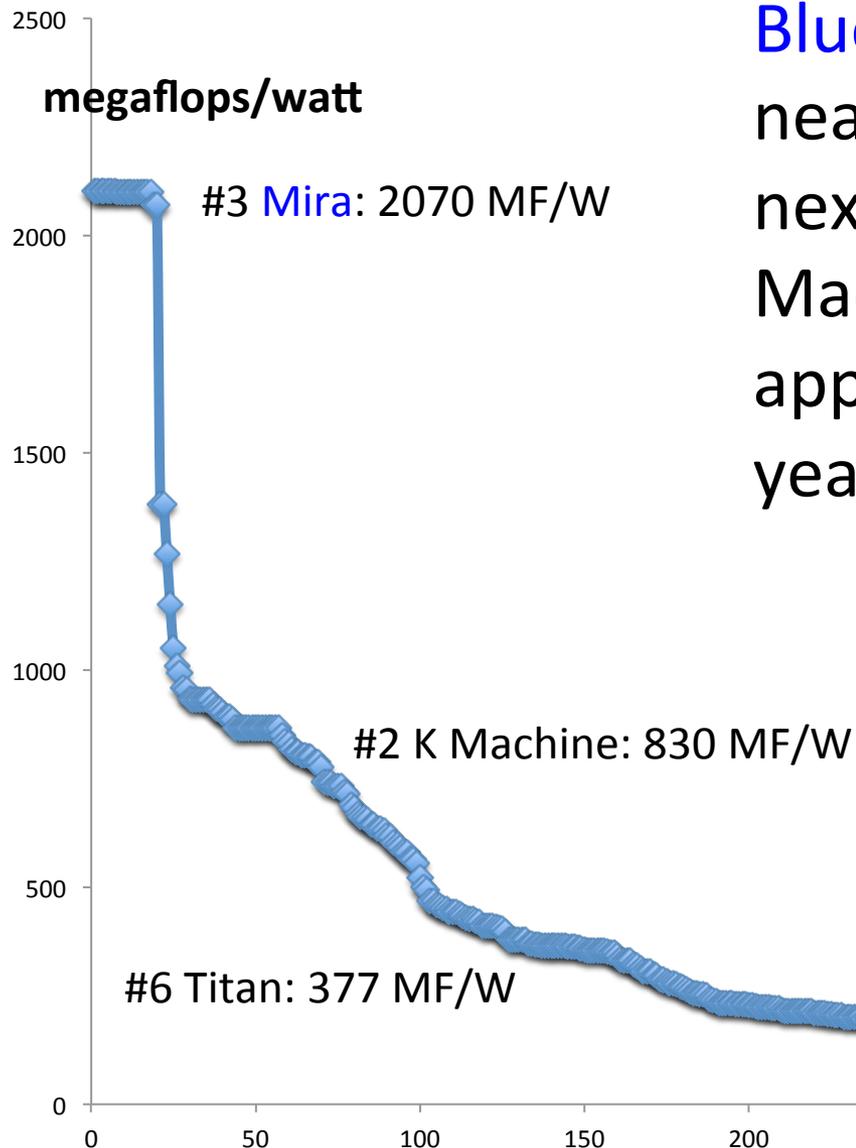


Efficiency

- Approximately 2% of all the power used in the United States is for data centers.
That's ten 1-gigawatt power plants!
- 1 MW per year costs approximately \$1,000,000.
- **Green500** measures the power efficiency of all known supercomputers in megaflop/s/watt (megaflop/s=1M math operations per second).
- A petaflop supercomputer uses megawatts...



Blue Gene/Q architecture is nearly 3x more efficient than the next best supercomputer (K Machine), saving DOE approximately 6MW and \$6M/year!



- Three generations of **Blue Gene**:

Blue Gene/L = 210 MF/W

Blue Gene/P = 378 MF/W

Blue Gene/Q = 2070 MF/W

- Three generations of **Toyota Prius**:

Prius 1.0 = 42/41 MPG

Prius 2.0 = 48/45 MPG

Prius 3.0 = 51/48 MPG

- If the Prius kept up with Blue Gene, it would achieve **400 miles per gallon!**



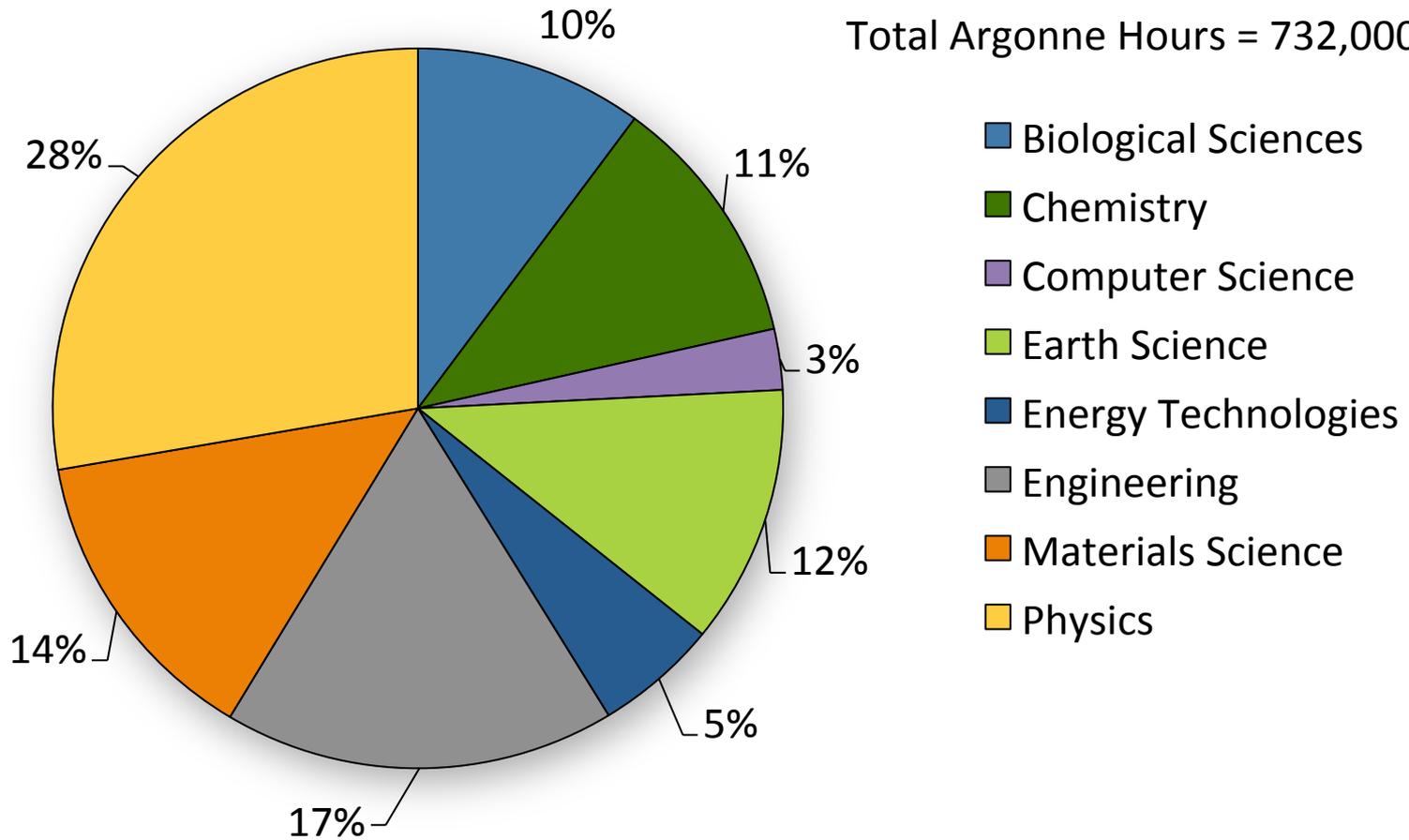
Science

- Supercomputers aren't just bigger...
- A desktop delivers 6000-8000 hours of computing a year.
- **Mira** will deliver 6,000,000,000 hours of computing a year.
- That's the same ratio as the distance to **Madison, WI** and the distance to **Mars!**



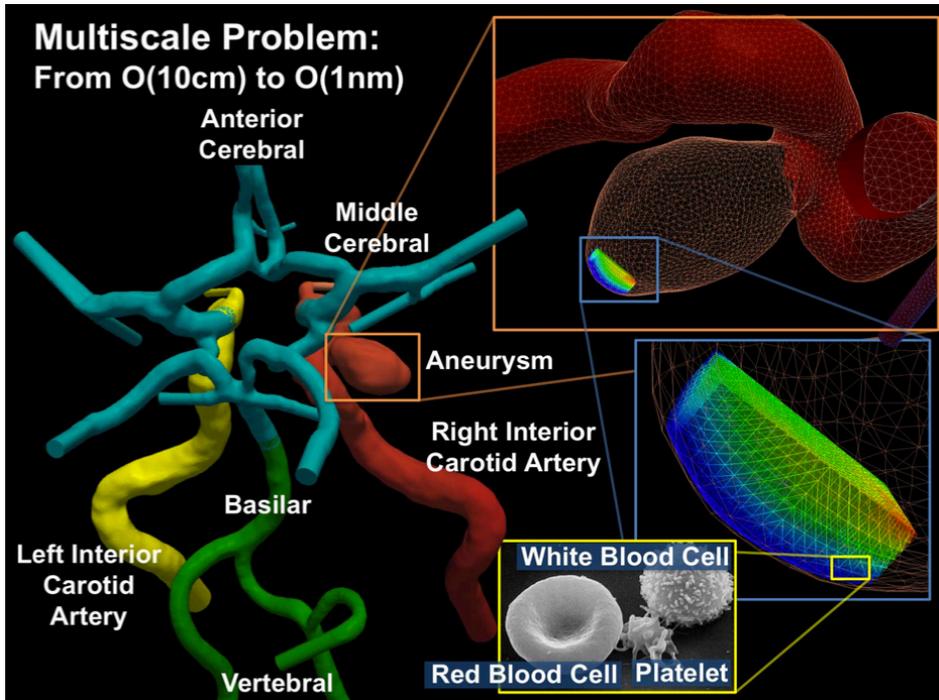
2011 INCITE Allocations by Discipline

Total Argonne Hours = 732,000,000

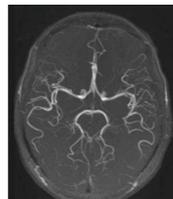


Multiscale Blood Flow Simulations

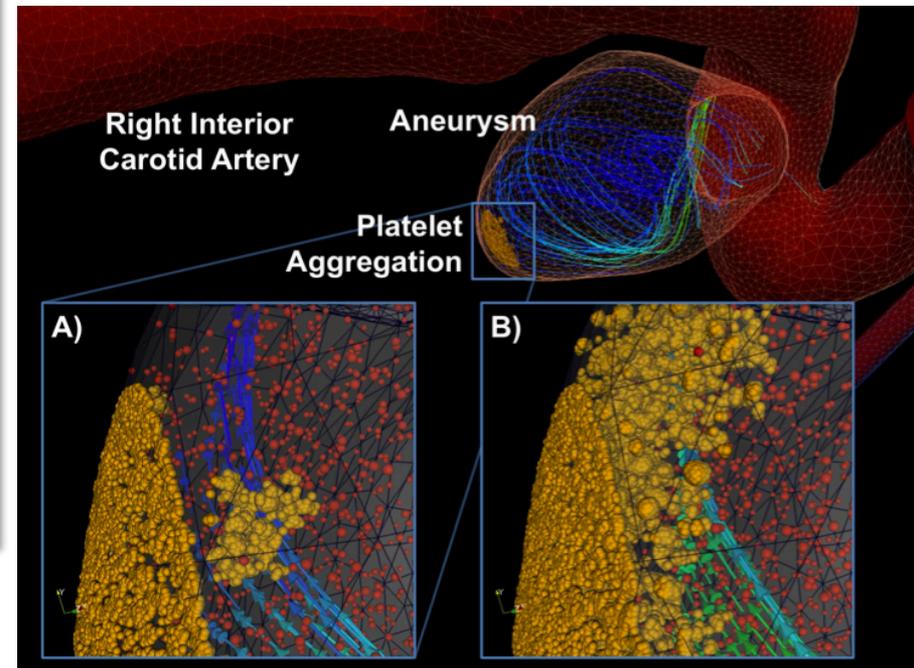
- **Approach:** multiscale simulations of the blood flow in the human brain vasculature: *arteries* (≥ 1 mm), *arterioles* (500-10 μm) and *capillaries* (5 μm).



Brain vasculature and aneurysm reconstructed from MRI images



Blood: RBC (45%), WBC (<1%), platelets (1%) and plasma



(A-B) Initial stages of clot formation and progress in time and space

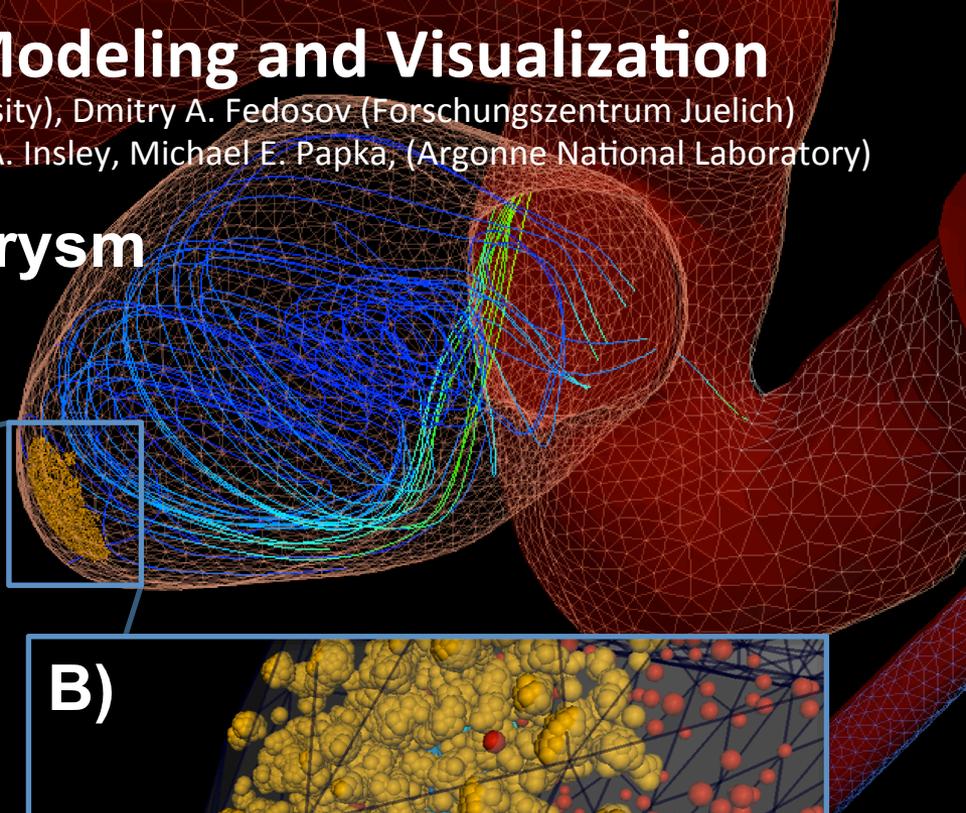
Blood Flow: Multi-scale Modeling and Visualization

Leopold Grinberg, George Karniadakis (Brown University), Dmitry A. Fedosov (Forschungszentrum Juelich)
Bruce Caswell (Brown University), Vitali Morozov, Joseph A. Insley, Michael E. Papka, (Argonne National Laboratory)

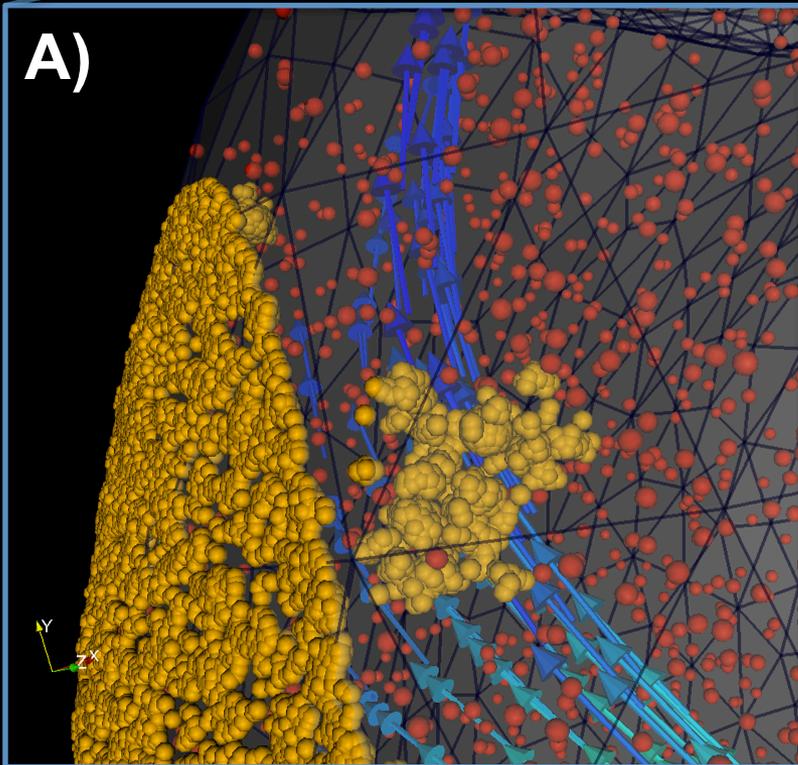
Right Interior
Carotid Artery

Aneurysm

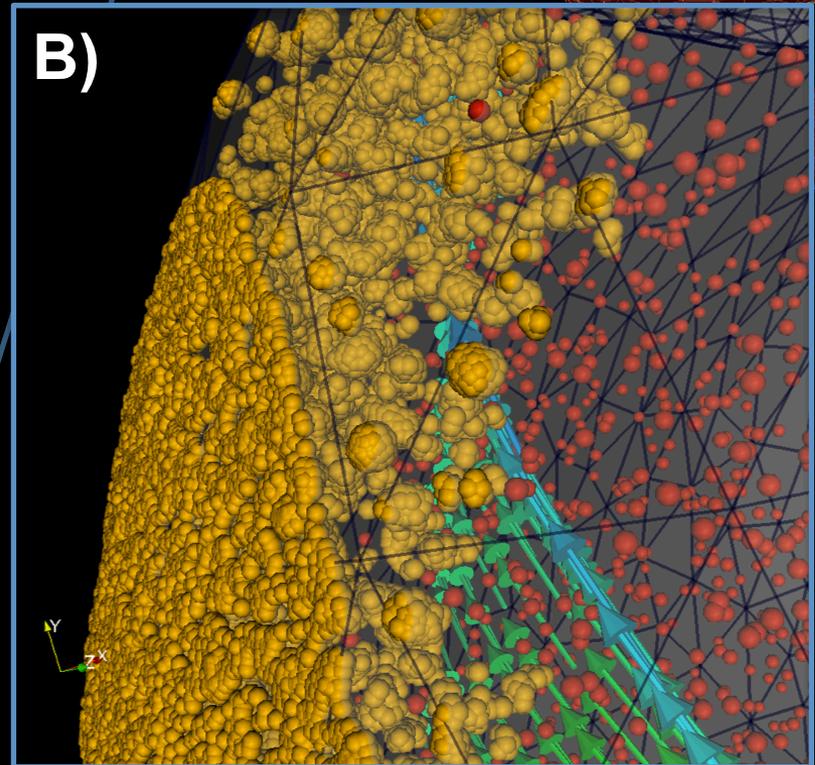
Platelet
Aggregation



A)



B)



Multiscale Blood Flow Simulations

Micro-domain: 3.93 mm³

DPD particles: 823,079,981

Results of a **24-hours simulation** on
32 racks of BG/P = 3.15M hours

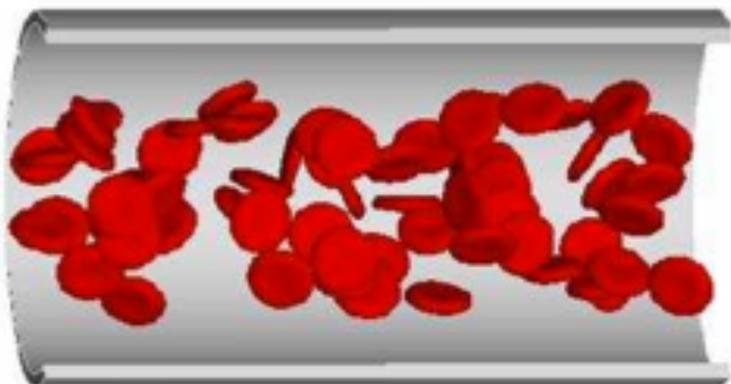
1 day x 80% of BG/P

= 3.15M CPU-hours

≈ 360 days ≈ **1 year** x 1 CPU

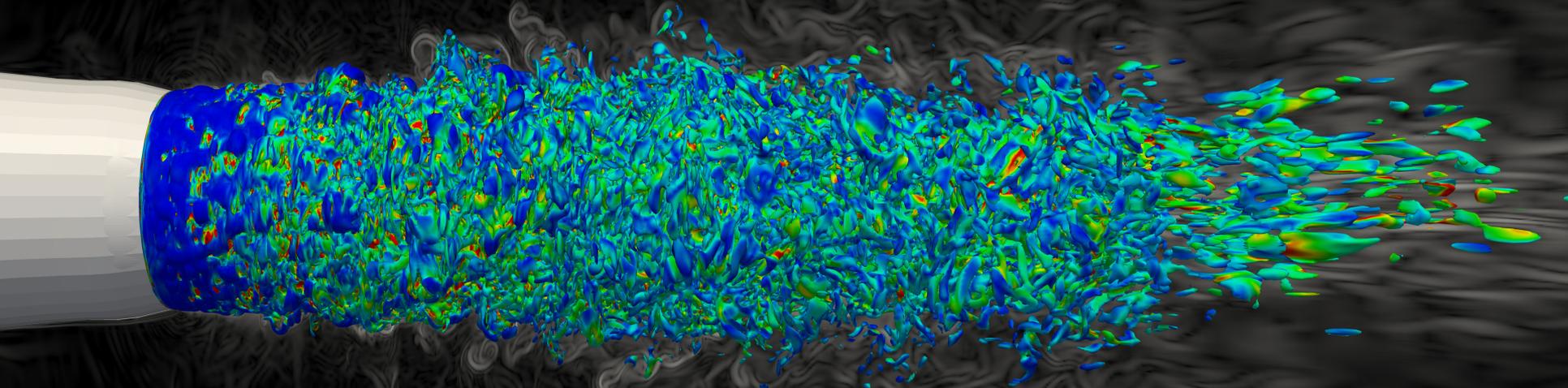
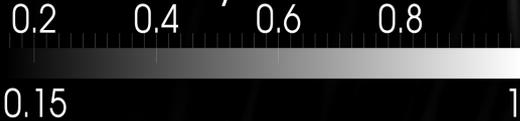
≈ 130,000 iterations

≈ **1/3 of a heart beat**



- **Cerebral aneurysms** occur in up to **5%** of the general population, leading to strokes for over **40,000** Americans each year.
- **Sickle cell (SS) anemia** (a chronic inflammatory disease) affects **72,000** individuals in USA.
- **Cerebral malaria (CM)** is a red blood cell (RBC) disease, with significant mortality. More than **1.5 Million deaths** each year – mostly in children.

Density Gradient



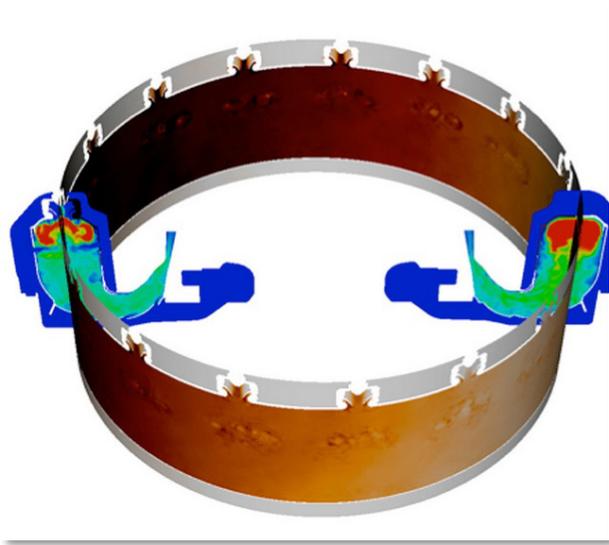
Vorticity Magnitude



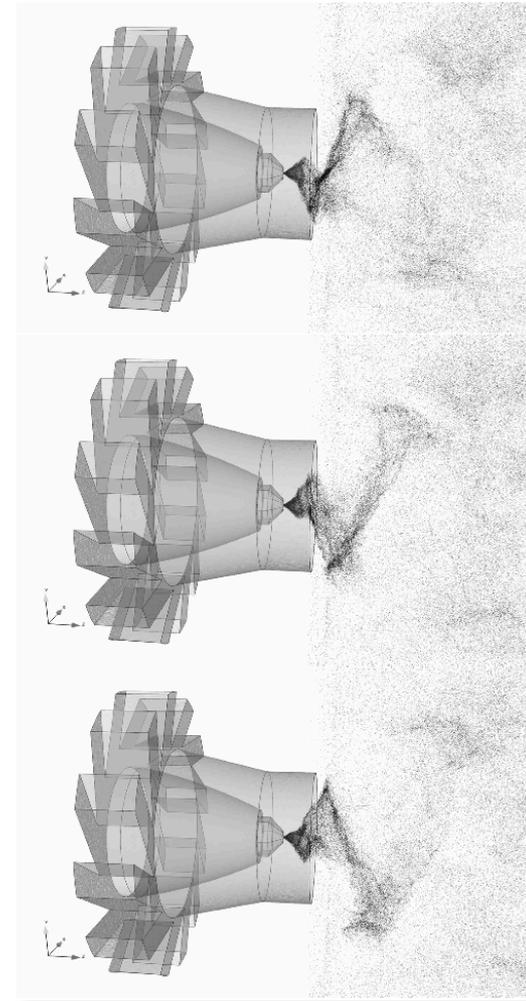
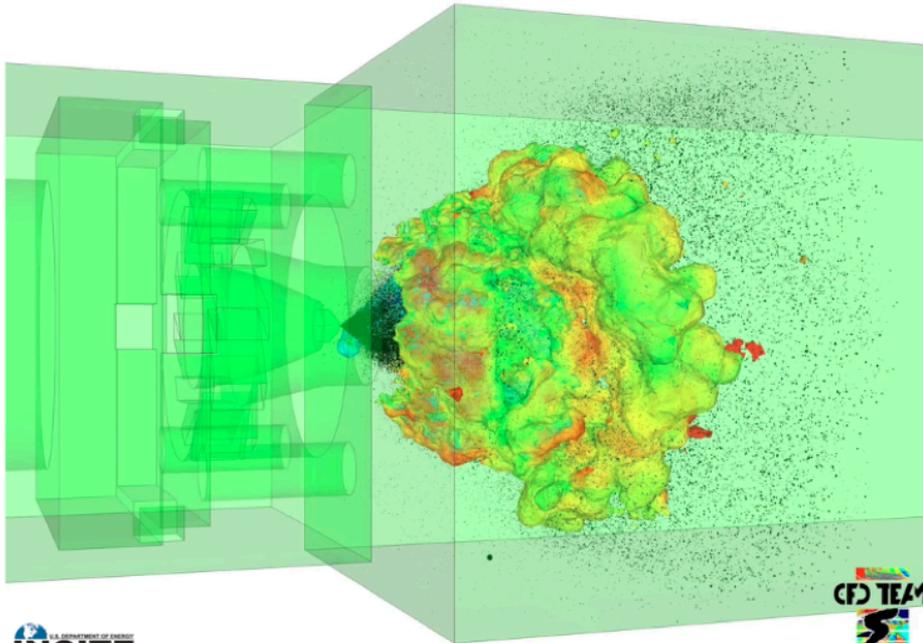
Turbulent Mixing Noise from Jet Exhaust Nozzles



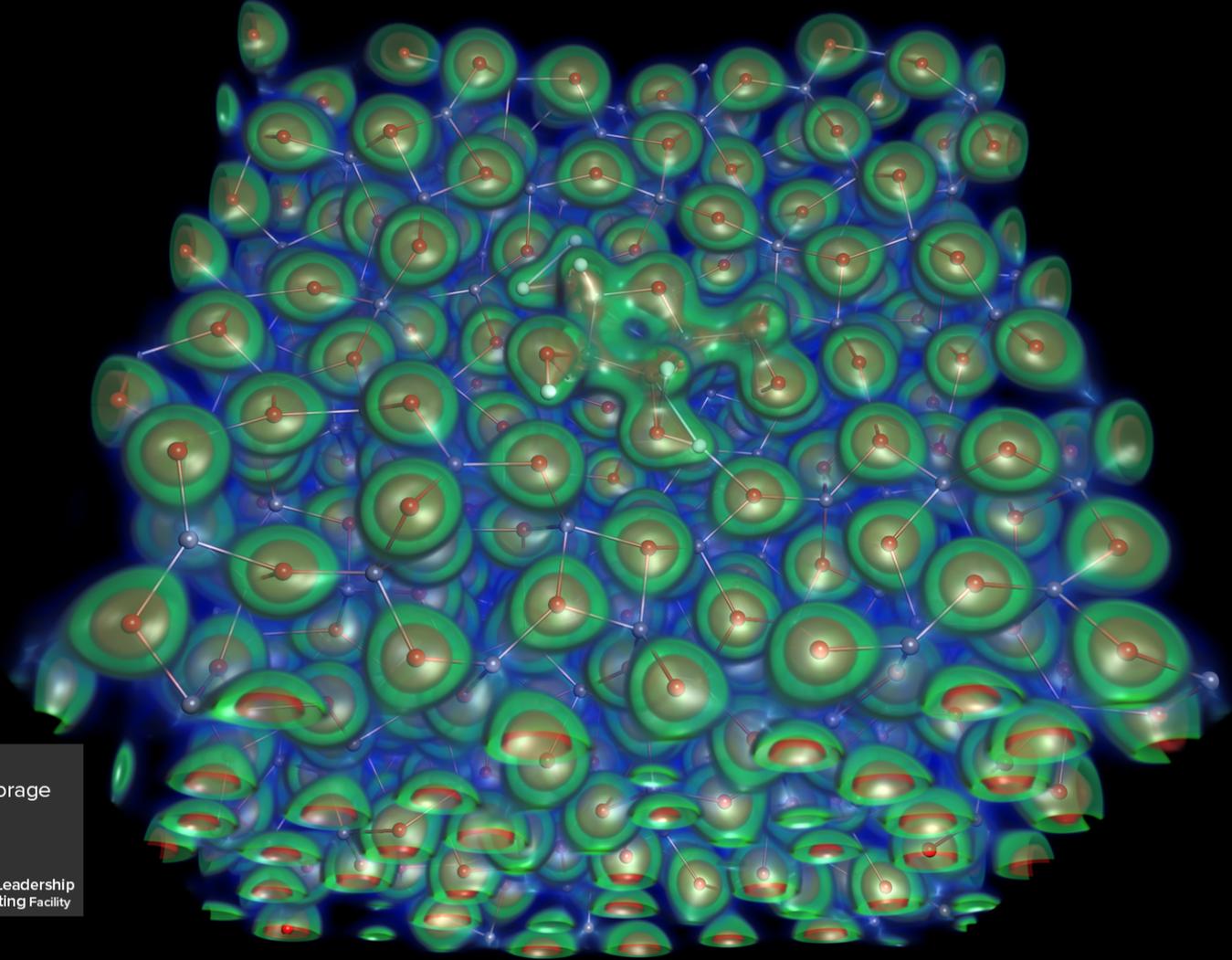
Simulation of Combustion in Gas Turbines



Fields of temperature and pressure in a simulation of a complete helicopter combustion chamber.



Visualization of the liquid particles with an industrial swirled injector



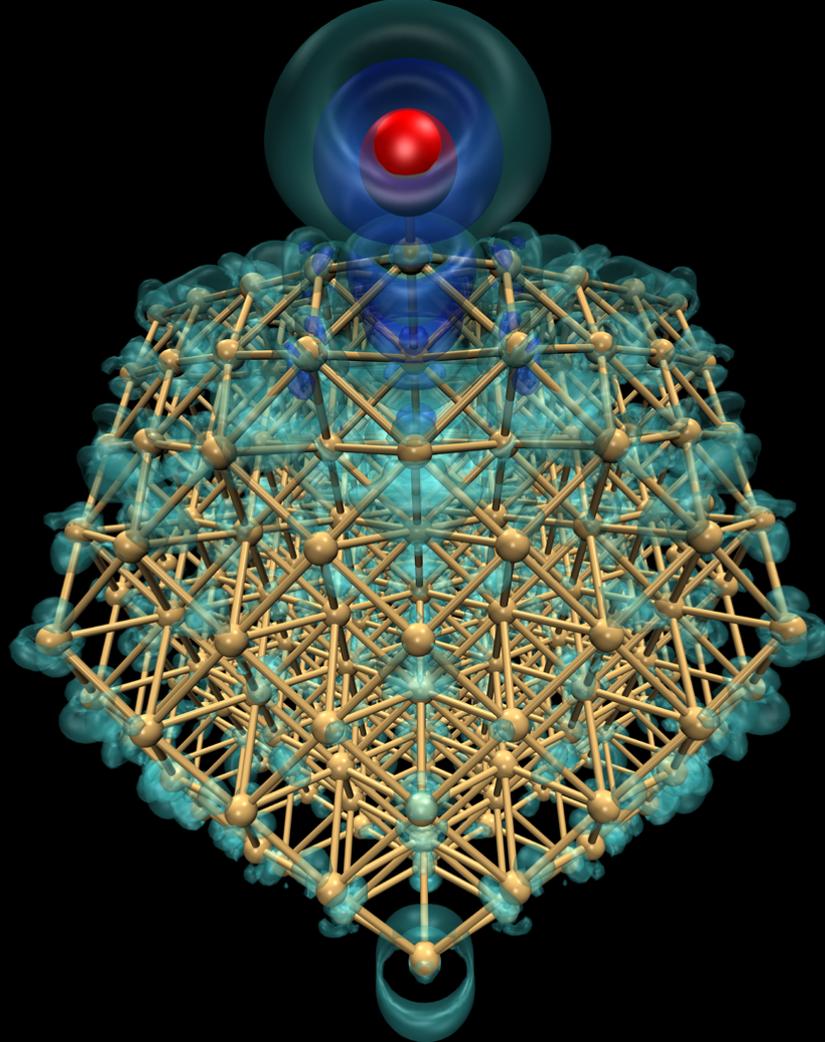
First Principles Calculations of
Interfaces in Electrical Energy Storage
Systems

PI: Larry Curtiss, Argonne National Laboratory



Efficient energy storage in batteries is critical to the development of cars and other vehicles that don't run on oil.

The important properties of batteries emerge at nanoscale or larger, which is thousands of atoms.



Probing the Non-scalable Nano Regime
in Catalytic Nanoparticles with Electronic
Structure Calculations

PI: Jeff Greeley, Argonne National Laboratory



Quantum mechanical simulations requires enormous amounts of memory, more memory than all the hard drives in your house.

Accurate modeling of catalytic properties of nanoparticles can't be done with less than a supercomputer.