OAK RIDGE National Laboratory

# Science on Summit and beyond


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U.S. DEPARTMENT OF ENERGY

# Reaching New Heights in Weather Forecasting's Exascale Future

*ECMWF and ORNL researchers use the power of Summit to simulate the Earth's atmosphere for a full season at 1-square-kilometer grid-spacing*

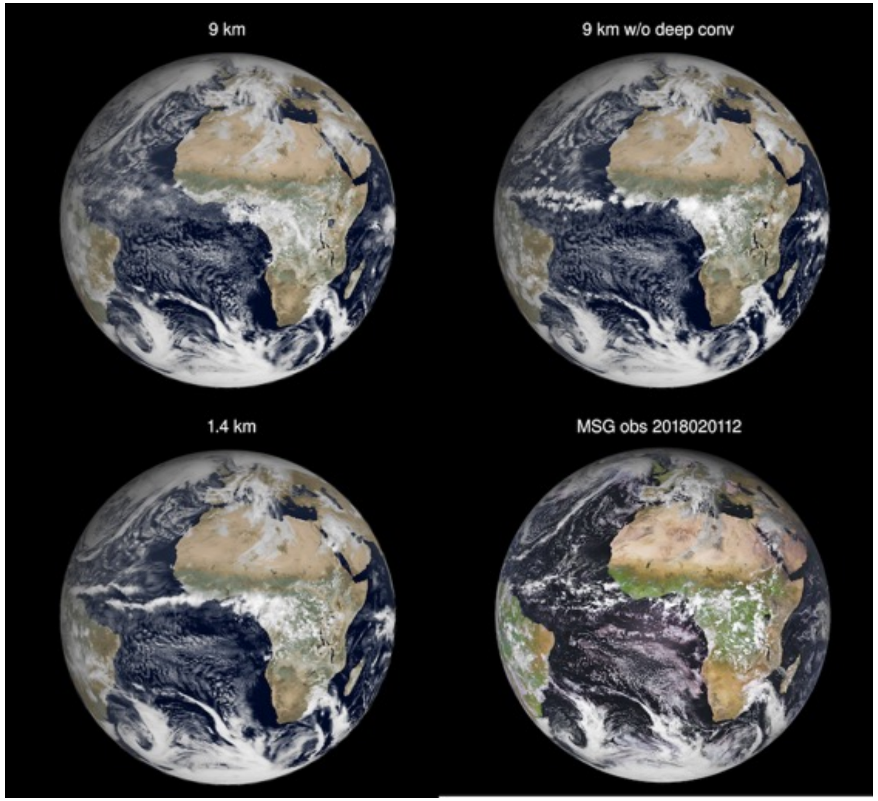
## The Science

Using Summit, a team of researchers from ECMWF and ORNL achieved a computational first: a global simulation of the Earth's atmosphere at a 1-square-kilometer average grid-spacing for a full 4-month season. Completed in June, the milestone marks a big improvement in resolution for the "European Model," which currently operates at 9-kilometer grid-spacing for routine weather forecast operations. It also serves as the first step in an effort to create multi-season atmospheric simulations at high resolution, pointing toward the future of weather forecasting—one powered by exascale supercomputers.

## The Impact

The team has made the simulation's data available to the international science community. By eliminating some of the fundamental modelling assumptions prevalent in conventional simulations, the high-resolution data may help to improve model simulations at coarser resolutions.

PI(s)/Facility Lead(s): Nils Wedi, ECMWF
ASCR Program/Facility: INCITE/OLCF
ASCR PM: Christine Chalk
Publication(s) related to this work: Wedi, N. P., et al. A baseline for global weather and climate simulations at 1 km resolution. *Journal of Advances in Modeling Earth Systems*, 12 (2020), e2020MS002192. doi: 10.1029/2020MS002192




*These simulated satellite images of Earth show the improvement in resolution of the ECMWF Integrated Forecasting System from 9-kilometer grid-spacing with parametrized deep convection (top left), to 9-kilometer grid-spacing (top right), and 1-kilometer grid-spacing (bottom left). On the bottom right is a Meteosat Second Generation satellite image at the same verifying time. Image courtesy ECMWF.*

# GE Spins up Supercomputer Models to Zero in on Energy Loss in Turbines

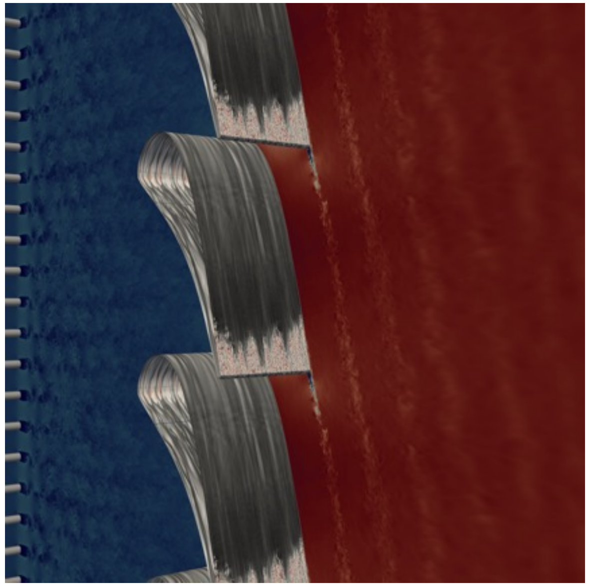
A team at GE Aviation and the University of Melbourne is studying turbulent flows on the Summit supercomputer for better engines

The Science

High-pressure turbines are vital components of gas turbines used to propel jet engines. The more efficient these jet engines are, the better they are for the aircraft industry and their customers. But these large, dynamic systems are difficult to study via experiments and physical testing. A team led by scientists at General Electric (GE) Aviation and the University of Melbourne used the Summit supercomputer to run for the first time real-engine cases capturing the largest eddies, or circular fluid movements, down to those that were tens of microns away from the turbine blade surface. From the simulations, the researchers determined which regions near a turbine blade experience a greater loss of energy. For the case with the highest Mach number, which describes the flow's velocity compared with the speed of sound, they discovered an extra loss of energy resulting from strong shock waves, or violent changes in pressure, that interact with the edge and wake of the flow to cause a massive amount of turbulence.

The Impact

More accurate prediction of real-engine conditions will lead to more efficient engines that consume less fuel and other positive derivative effects. A 1 percent reduction in fuel consumption across a fleet of engines is equal to about 1 billion dollars a year in fuel cost savings. Reduced fuel consumption also translates into reduced emissions—a 1 percent reduction in fuel burn reduces $CO_2$ emissions by roughly 1.5 percent.



*A row of upstream bars produces highly turbulent flow that gets accelerated through a high-pressure turbine blade row and interacts with the blade surface, causing significant temperature variations. Image Credit: Richard Sandberg, University of Melbourne*

PI(s)/Facility Lead(s): Richard Sandberg, Univ. Of Melbourne; Sriram Shankaran, GE Aviation
ASCR Program/Facility: INCITE/OLCF
ASCR PM: Christine Chalk
Publication(s) for this work: Y. Zhao and R. D. Sandberg, "High-Fidelity Simulations of a High-Pressure Turbine Vane," *Journal of Turbomachinery* 143, no. 9 (2021).

Y. Zhao and R. D. Sandberg, "Using a New Entropy Loss Analysis," *Journal of Turbomachinery* 142, no. 8 (2020): 081008

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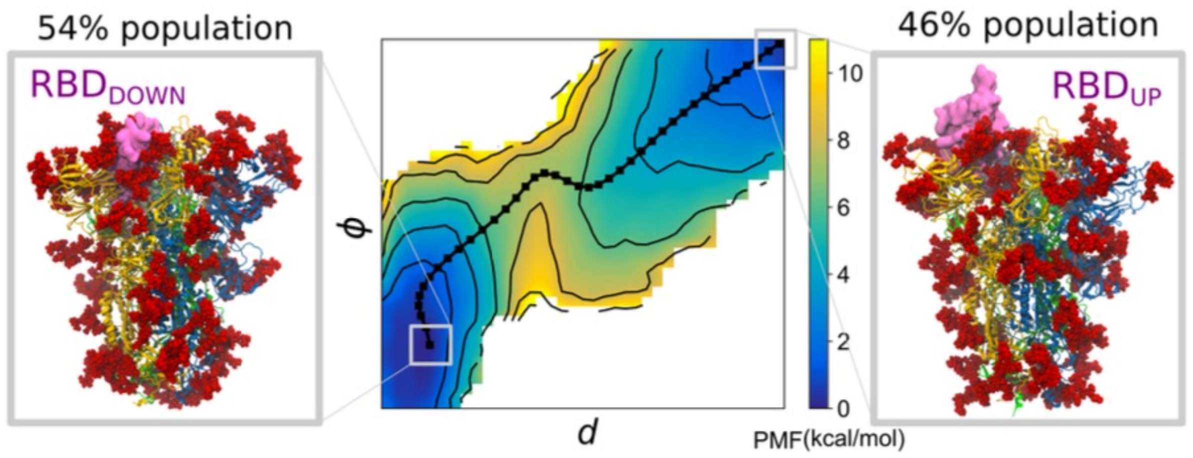
The University of Melbourne

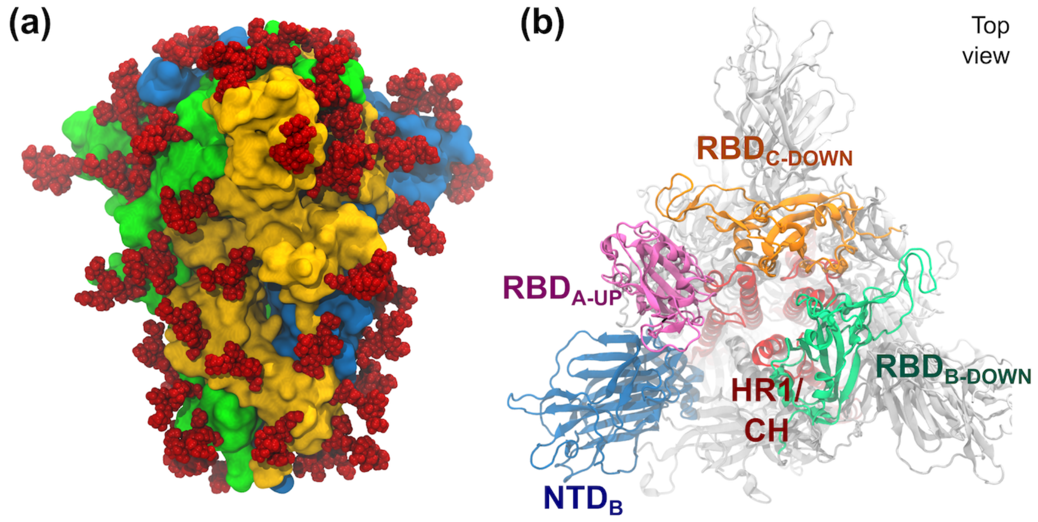
GE Aviation

INCITE

## Determining The Contribution of Glycosylation To SARS-CoV-2 S-protein Conformational Dynamics (PI: James Gumbart, Ga. Tech)

- Study of the conformational transition of the SARS-CoV-2 spike protein from a closed, noninfectious state to an open one that can bind to its receptor ACE2 on human cells and the role of glycans in function.
- One antibody's (BD-368-2) epitope is exposed regardless of whether the S-protein is in the up or down state (Yu et al. https://doi.org/10.1101/2021.08.12.456168)



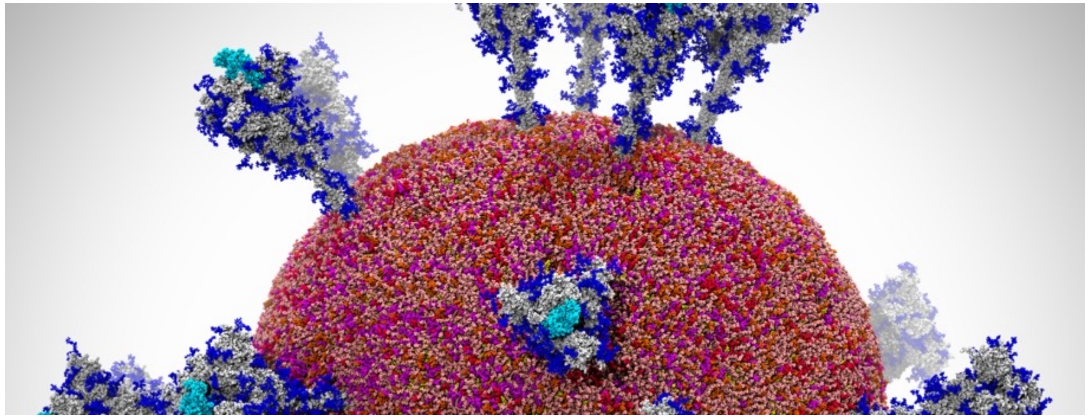



# Gordon Bell Special Prize-Winning Team Reveals AI Workflow for Molecular Systems in the Era of COVID-19 (PI: Rommie Amaro, UCSD)

Research by team at ANL and UC San Diego leads to a novel understanding of SARS-CoV-2 and a new method for studying disease

## The Science

Imaging techniques, such as X-ray imaging and cryogenic electron microscopy, can provide snapshots of viruses such as SARS-CoV-2, but these fall short of capturing the dynamic movements of viral proteins. Computer simulations can help scientists capture the movements of these structures virtually. Now, a team led by Rommie Amaro at the University of California San Diego and Arvind Ramanathan at ANL have built a first-of-its-kind workflow based on AI and have run it on OLCF's Summit supercomputer to simulate the virus's spike protein in numerous environments, including within the SARS-CoV-2 viral envelope comprising 305 million atoms—the most comprehensive simulation of the virus performed to date. The accomplishment has earned the ACM Gordon Bell Special Prize for HPC-Based COVID-19 Research.



*A snapshot of a visualization of the SARS-CoV-2 viral envelope comprising 305 million atoms. Image Credit: Rommie Amaro, UC San Diego; Arvind Ramanathan, ANL*

## The Impact

The team was able to successfully scale NAMD to 24,576 of Summit's NVIDIA V100 GPUs. The results of the team's initial runs on Summit have led to discoveries of one of the mechanisms that the virus uses to evade detection as well as a characterization of interactions between the spike protein and the protein that the virus takes advantage of in human cells to gain entry—the ACE2 receptor. The team is now integrating their scientific code, NAMD, into their workflow pipeline to fully automate the transition from simulation to AI for data processing without gaps.

PI(s)/Facility Lead(s): Rommie Amaro
ASCR Program/Facility: INCITE / OLCF
ASCR PM: Christine Chalk
Publication(s) for this work: Lorenzo Casalino, Abigail Dommer, Zied Gaieb, Emilia P. Barros, Terra Sztain, Surl-Hee Ahn, Anda Trifan, Alexander Brace, Anthony Bogetti, Heng Ma, Hyungro Lee, Matteo Turilli, Syma Khalid, Lillian Chong, Carlos Simmerling, David J. Hardy, Julio D. C. Maia, James C. Phillips, Thorsten Kurth, Abraham Stern, Lei Huang, John McCalpin, Mahidhar Tatineni, Tom Gibbs, John E. Stone, Shantenu Jha, Arvind Ramanathan, and Rommie E. Amaro. "AI-Driven Multiscale Simulations Illuminate Mechanisms of SARS-CoV-2 Spike Dynamics." *International Journal of High-Performance Computing Applications, SC20*( 2020).

# In 2021, Frontier will become the nation's first exascale computer



| FRONTIER | |
|---|---|
| Peak Performance | >1.5 EF |
| Node | 1 HPC and AI-optimized AMD EPYC CPU + 4 purpose-built AMD Radeon Instinct GPU |
| Memory | Approximately 10 PB of combined high bandwidth and DDR memory |
| On-node Interconnect | AMD Infinity Fabric<br>Coherent memory across the node |
| System Interconnect | Cray four-port Slingshot network<br>100 GB/s |
| Topology | Dragonfly |
| Storage | 2-4x performance and capacity of Summit's I/O subsystem. |
| Node-local NVMe | Yes |


Daniel Kasen, Ann Almgren, Don Wilcox, Wick Haxton (LBNL)

Philipp Mösta, Ken Shen (Berkeley)

Bronson Messer, Raph Hix, Eirik Endeve, Anthony Mezzacappa, Austin Harris, Ran Chu, Eric Lentz, Michael Sandoval, Fernando Rivas (ORNL/UTennessee)

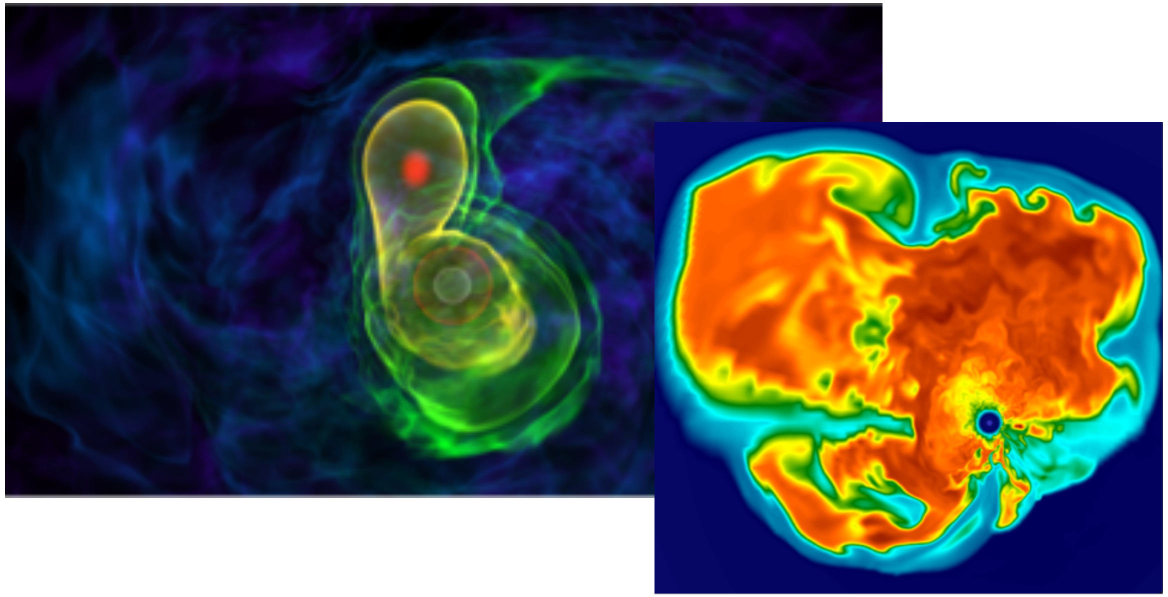
Sean Couch, Michael Pajkos, Jennifer Ranta (Michigan State)

Anshu Dubey, Saurabh Chawdhary, Carlo Graziani, Jared O’Neal (ANL)

Klaus Weide (UChicago)

Mike Zingale, Xinlong Li (Stony Brook)

- ExaStar simulations are essential to:
  - Guide future nuclear physics experimental programs
    - siting the r-process directly impacts which rates are most important to measure
  - Provide reliable templates for gravitational wave and neutrino detectors
    - Low signal-to-noise requires templates for matching
  - Interpret X-ray and gamma-ray observations



- ExaStar simulations will have connections to:
  - experimental nuclear physics data
  - satellite observations of astrophysical phenomena
  - GW detections
  - neutrino experimental data, including solar and reactor experiments to improve predictive power

DEEP UNDERGROUND NEUTRINO EXPERIMENT