

Office of Science 2021 DISTINGUISHED SCIENTIST FELLOWS CEREMONY

Virtual Ceremony October 2021



THE UNITED STATES DEPARTMENT OF ENERGY OFFICE OF SCIENCE

Welcomes you to the 2021 Distinguished Scientist Fellows Award Ceremony

The 2021 DOE Office of Science Distinguished Scientist Fellows are:

Gregory W. Hammett of Princeton Plasma Physics Laboratory

For leading the development of the quantitative theory and simulation of plasma turbulence in fusion and astrophysics, and for educating and mentoring a diverse group of graduate students and early career researchers.

Jay Keasling of Lawrence Berkeley National Laboratory

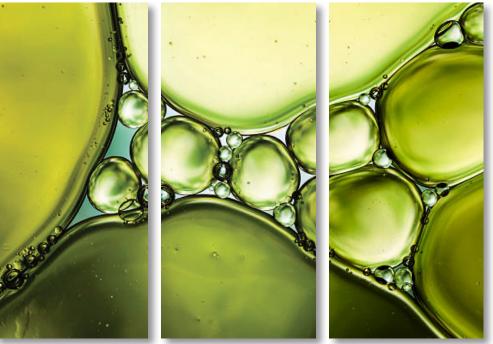
For national scientific leadership in synthetic biology that has advanced DOE's strategy in renewable energy, especially the realization of biofuels and bioproducts that enable biomanufacturing at scale, and inspire and grow the U.S. bioeconomy.

L. Ruby Leung of Pacific Northwest National Laboratory

For pioneering new approaches in climate modeling, the discovery of unexpected impacts of regional climate change, and understanding extreme weather events and their future changes.



AGENDA



Introductory Remarks

David Turk Deputy Secretary of Energy

Award Conferment

J. Stephen Binkley Acting Director Office of Science

Brief Remarks from the 2021 Fellows

Gregory W. Hammett Princeton Plasma Physics Laboratory

Jay Keasling Lawrence Berkeley National Laboratory

L. Ruby Leung Pacific Northwest National Laboratory

Roundtable Q&A with the 2021 Fellows

Harriet Kung Deputy Director for Science Programs Office of Science

2021 FELLOWS

Dr. Gregory W. Hammett Princeton Plasma Physics Laboratory

Dr. Jay Keasling Lawrence Berkeley National Laboratory

Dr. L. Ruby Leung Pacific Northwest National Laboratory





GREGORY W. HAMMETT

Princeton Plasma Physics Laboratory

Dr. Greg Hammett is a Principal Research Physicist at the Princeton Plasma Physics Laboratory (PPPL), a US Department of Energy National Laboratory. He is also a Lecturer with Rank of Professor in the Princeton University Program in Plasma Physics, and is part of the associated faculty of the Program in Applied and Computational Mathematics. He became a Fellow of the American Physical Society in 1997. A child of the Apollo moon landing era, he got interested in physics through his father, a US Air Force fighter pilot, and through Star Trek reruns and popular science books. He graduated from Baldwin County High School in Milledgeville, Georgia in 1976, in the middle of the first energy crisis, and at that time got interested in fusion energy. He graduated from Harvard in 1980, finished his Ph.D. in plasma physics from Princeton in 1986, and has worked at PPPL since, though assignments included the European JET tokamak, Imperial College London, Berkeley, and Oxford. PPPL does research in plasma physics and fusion energy, which has the potential to be an attractive new energy source. Dr. Hammett specializes in computational and theoretical studies of the complex physics of plasma turbulence. He and collaborators are working on supercomputer simulations of 5-dimensional gyrokinetic plasma turbulence in fusion devices, and are studying methods to reduce turbulent heat losses, which could lead to a more economical fusion power plant. Most recently, they have been working on a code using novel versions of Discontinuous Galerkin algorithms for the challenging edge region of tokamaks. His work on fluid models of Landau-damping (which extends fluid equations to low collisionality where traditional closure approximations break down) has been cited in over 400 papers, finding application to diverse fields such as MHD turbulence in astrophysical plasmas, plasma processing of semiconductors, laser-plasma interactions, and his own specialty of fusion devices. He has done some astrophysics, such as kinetic effects on magnetorotational instability turbulence in accretion disks around black holes. He has supervised 12 Ph.D. students, and thanks his students and colleagues for the many things he has learned from them.



AWARD ABSTRACT

Using Supercomputers and Advanced Algorithms to Understand Aspects of Turbulence in Fusion Power Plants

by Dr. Gregory W. Hammett

Fusion energy is one of the most difficult scientific and engineering challenges humans have undertaken. Fusion is among the few long-term options that can provide a reliable, stable energy source needed to offset the intermittent nature of solar power and other sources. Some exciting ideas are being pursued in the U.S. and worldwide that could lead to more attractive fusion power plants, though challenges remain, and much work is needed to test these ideas and turn them into reality. Such ideas include using liquid lithium metal to reduce plasma turbulence and help handle the enormous heat fluxes from a fusion reactor, innovative magnetic geometries for tokamak and stellarator fusion devices to confine plasmas, and advances in superconductors.

DOE scientists have long been at the forefront of using supercomputers to advance fusion research and other sciences. Supercomputers are now a million times more powerful than 25 years ago (when many present scientists were in college), enabling simulations of unparalleled capability that were inconceivable then. But fusion devices are highly complicated, involving many physical effects interacting at a wide range of scales, so just having superfast computers is not enough. A lot of work is ongoing to develop complex physical models with sufficient fidelity; to identify or invent efficient algorithms; to translate all of this into efficient codes for solving these equations; and finally, to test these codes by comparing them with experiments.

This project aims to contribute to the U.S. fusion program by focusing on four important tasks that are somewhat speculative but may have a significant payoff. One task is to apply a cutting-edge plasma turbulence code to try to understand the dramatic reduction in turbulence with lithium being studied in the LTX-beta experiment at PPPL, and how this improvement might extrapolate to reactor scales. We will use the Gkeyll code (which uses versions of Discontinuous Galerkin algorithms) under development by a team at PPPL and

collaborators. A second task is to study certain subtle theoretical issues underlying global gyrokinetic codes, such as how one might improve boundary conditions for higher-order drifts of ions. A third is to investigate possible multi-scale algorithms for parts of the calculations to significantly speed up these codes. Finally, we will explore some speculative ideas on how to improve reduced transport models. These models can be used for faster evaluation inside optimization loops for fusion reactor design codes and would be designed to handle general complex magnetic geometries to aid the study of novel shapes for both tokamaks and stellarators.

This project will encourage scientific exchanges by supporting postdocs and graduate students, at PPPL, Princeton University, the University of Maryland, and via summer graduate interns from other universities. It will build on existing collaborations in the Gkeyll group that also involve MIT, Virginia Tech, the University of Texas, the University of Iowa, General Atomics, and others. Overall, this project will contribute to the study of methods to reduce small scale turbulence that causes hot particles to leak out of a fusion device. Reducing turbulence could significantly improve fusion performance and lead to more attractive fusion power plants.

JAY KEASLING

Lawrence Berkeley National Laboratory

Jay Keasling is a senior faculty scientist at Lawrence Berkeley National Laboratory, the Philomathia Distinguished Professor of Alternative Energy at the University of California, Berkeley in the Department of Bioengineering and the Department of Chemical and Biomolecular Engineering, and Chief Executive Officer of the Joint BioEnergy Institute (JBEI). Dr. Keasling's research focuses on metabolic engineering of microorganisms for environmentally friendly synthesis of drugs, chemicals, and fuels. Keasling received a B.S. in Chemistry and Biology from the University of Nebraska and M.S. and Ph.D. in Chemical Engineering from the University of Michigan and did post-doctoral research in biochemistry at Stanford University. He is a member of the National Academy of Engineering, the National Academy of Inventors, and the American Academy of Arts and Sciences. Keasling has published over 500 papers in peer-reviewed journals, has over 65 issued patents, and has won numerous awards. Keasling is the founder of Amyris, LS9, Lygos, Napigen, Demetrix, Maple Bio, Apertor Pharma, and Zero Acre Farms.



AWARD ABSTRACT

Structure-based engineering of polyketide synthases for production of biofuels and bioproducts by Jay Keasling

We propose to develop a protein structure-based platform for engineering large protein complexes called polyketide synthases (PKSs) for synthesis of biofuels and bioproducts. We will use the latest advances in protein structure prediction (e.g., AlphaFold and RoseTTAFold) and determination (cryoelectron microscopy and small angle X-ray scattering) to elucidate structures for a set of natural and engineered PKS modules that will be the most useful in producing highly reduced hydrocarbons and polymer monomers. We will develop an interface between our PKS design software and AlphaFold/RoseTTAFold to allow incorporation of protein structures into existing PKS design software to enable structure-based design of PKSs.

We will demonstrate the utility of the structurebased design for production of renewable, carbon-neutral gasoline, diesel, and jet fuels. This work is made possible by access to several, unique DOE User Facilities including the National Energy Research Scientific Computing Center (NERSC), the CryoTEM facilities at the Environmental Molecular Sciences Laboratory (EMSL) at Pacific Northwest National Laboratory, and the SIBYLS (Structurally Integrated BiologY for the Life Sciences) small angle X-ray scattering beamline at the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory.

This work will lay the foundation for structurebased design of PKSs and their use for synthesis of many carbon-neutral, renewable biofuels and bioproducts from forest and agricultural waste. Because the fuels will be made from plant materials, no additional carbon will be added to the atmosphere when they are burned, which will reduce the impact of fuel use on global climate change.

L. RUBY LEUNG

Pacific Northwest National Laboratory

L. Ruby Leung is a Battelle Fellow at Pacific Northwest National Laboratory. Her research broadly cuts across multiple areas in modeling and analysis of climate and water cycle including orographic precipitation, monsoon climate, extreme events, land surface processes, land-atmosphere interactions, and aerosol-cloud interactions.

Ruby is the Chief Scientist of the U.S. Department of Energy (DOE)'s Energy Exascale Earth System Model (E3SM), a major effort to develop state-of-the-art capabilities for modeling human-Earth system processes on DOE's next generation high performance computers. She is also the principal investigator of the DOE Water Cycle and Climate Extreme Modeling (WACCEM) science focus area that is pioneering research in understanding and modeling variability and changes in precipitation and hydroclimatic extremes in a warming climate.

She has organized many workshops sponsored by Department of Energy, National Science Foundation, National Oceanic and Atmospheric Administration, and National Aeronautics and Space Administration to define gaps and priorities for climate research. Ruby is a member of the Board on Atmospheric Sciences and Climate (BASC), National Academies of Sciences, Engineering, and Medicine and an editor of the American Meteorological Society (AMS) Journal of Hydrometeorology and American Geophysical Union (AGU) Journal of Geophysical Research-Atmospheres. She is also a council member of AMS and a board member of Washington State Academy of Sciences.

Ruby is an elected member of the National Academy of Engineering and Washington State Academy of Sciences and a fellow of the AMS, AGU, and American Association for the Advancement of Science (AAAS). She is the recipient of the 2019 AGU Global Environmental Change Bert Bolin Award and Lecture and the 2020 AGU Atmospheric Science Jacob Bjerknes Lecture. She has been selected for the 2022 AMS Hydrologic Sciences Medal for her "ingenious, groundbreaking contributions which enhance the modeling of land-atmosphere interactions and the hydroclimate." Ruby has published over 375 papers in peer reviewed journals. She received a BS in Physics and Statistics from Chinese University of Hong Kong and an MS and PhD in Atmospheric Sciences from Texas A&M University.







AWARD ABSTRACT

North American Hydroclimate: East-West Contrasts and Connections by L. Ruby Leung

Eastern and western North America feature largely contrasting geography and hydroclimate with humid conditions in the east and arid climate in large parts of the west. These regions are also marked by pronounced differences in precipitation seasonality and flood- producing storm types. Demarcation of eastern and western North America by the Continental Divide separating watersheds that drain into the Atlantic Ocean vs. the Pacific Ocean further highlights the unique characteristics of the two regions. Hence previous studies of North American hydroclimate have mainly focused on the characteristics of the eastern and western regions separately, leaving important gaps in understanding and modeling the connections between the regions. With western North America located upstream of the east, there are obvious connections between the two regions particularly in the presence of the western mountains that provide mechanical and thermal forcing that influences atmospheric circulation and convection downstream. However, even the eastern region may influence the western region by exciting circumglobal stationary waves that induce subsidence and drying over the western region.

Recognizing the many physical and dynamical mechanisms through which the hydroclimate of eastern and western North America are connected, this proposal aims to fill important gaps in understanding and modeling the hydroclimate and extreme events of North America by focusing on hydroclimate elements contrasting and connecting the two regions. More specifically, we will address two key sets of science questions: (1) What are the sources of eastward propagating sub-synoptic disturbances that trigger mesoscale convective systems in the Great Plains during summer? How may model limitations in simulating these disturbances contribute to the prevalent summer warm-dry biases in Central U.S. in regional and global climate models? What are the implications for predictability of warm-season hydrologic extremes in eastern U.S.? How might changes in the eastward propagating disturbances contribute to changes in mesoscale convective systems under global warming? (2) How might extreme events in western and eastern North America be synchronized by regional-to-continental scale processes and global teleconnections? What physical and dynamical processes underline the synchronization? How well can climate models capture the synchronization? How might the synchronization be modulated by global warming? These questions will be addressed using newly available high-resolution datasets, regional and global convection permitting models including the Energy Exascale Earth System Model (E3SM), and complex network analysis and machine learning approaches, with the goal of improving understanding and modeling of extreme events and their precursors and synchronization that contribute to earth system predictability.



THE OFFICE OF SCIENCE DISTINGUISHED SCIENTIST FELLOWS

2020 Jacqueline Chen Sandia National Laboratories/California



For advancing frontiers in the fields of combustion and highperformance computing through petascale direct numerical simulations and for mentoring and inspiring generations of researchers.

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James De Yoreo Pacific Northwest National Laboratory



For transformational discoveries that have reshaped our understanding of materials synthesis from complex nucleation pathways to hierarchical assembly, for leadership in National Laboratory-University partnerships, and for dedication to mentoring the next generation of scientists.

2020 Cynthia Keppel Thomas Jefferson National

Accelerator Facility



For contributions to the exploration of the quark structure of hadrons and nuclei through electron scattering, and creating successful collaborations across disciplines, including electron and neutrino scattering, theory and experiment, and nuclear and medical applications.

2019 Ian Foster Argonne National Laboratory



For trailblazing work in distributed and high performance computing with fundamental and long-lasting impacts on both computer science as a discipline and the practice of computing across the Office of Science.

2019 Barbara Jacak Lawrence Berkeley National Laboratory



For leadership in discovering and characterizing the hottest, densest matter in the universe - the quark gluon plasma - and in building collaborations and training scientists at the frontiers of nuclear physics. 2019 Sally Dawson Brookhaven National Laboratory



2019 Joshua Frieman Fermi National Accelerator Laboratory



2019 José Rodriguez Brookhaven National Laboratory



For transformational discoveries that have reshaped our understanding of materials synthesis from complex nucleation pathways to hierarchical assembly, for leadership in National Laboratory-University partnerships, and for dedication to mentoring the next generation of scientists.

For pioneering advances in the science of dark energy and cosmic acceleration, including leading the Sloan Digital Sky Survey-II Supernova Survey, co-founding the Dark Energy Survey and service as its Director.

For discoveries of the atomic basis of surface catalysis for the synthesis of sustainable fuels, and for significantly advancing in-situ methods of investigation using synchrotron light sources.

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