Introduction to the Session: Animal Linguistics: Origins and Evolution of Language: Some Things Never Change: An Ethological Approach to Investigating The Origins of Humpback Whale Vocal Behavior

Michelle Fournet, University of New Hampshire

Communication is key for all social animals. In the marine environment, where light attenuates quickly but sound travels great distance with little loss of energy, acoustic communication has emerged as the primary sensory modality for maintaining contact between individuals. Humpback whales (Megaptera novaeangliae) are a globally distributed baleen whale species well known for their diverse acoustic behavior and complex social structure. Breeding age male whales produce ‘song’, an intricate and stereotyped acoustic display associated with reproduction, while whales of all age and sex class produce ‘calls’ throughout their migratory range. Despite decades of research on humpback whale song, investigation into the role of calls in the ecology of humpback whales is relatively new. Contrasting the two communication modalities presents an opportunity to understand the foundation for the evolution of humpback whale acoustic behavior. In this presentation, I will contrast research focused on ephemeral yet stereotyped male singing behavior on breeding grounds, with the more ubiquitous and stable calling behavior of humpback whales on foraging grounds. I will address drivers of humpback whale vocal behavior (innate calls vs. culturally transmitted song), call function, how humpback whales adjust call patterns in response to the marine soundscape, and how the changing acoustic habitat of whales in the Anthropocene may result in shifts in humpback whale acoustic communication.

Linking Communication and Cooperation – Lessons from the Naked Mole-Rat

Alison Barker, Max Planck Institute for Brain Research

Highly organized social groups require well-structured and dynamic communication systems. Naked mole-rats form some of the most rigidly structured social groups in the Animal Kingdom, exhibiting eusociality, a type of highly cooperative social living characterized by a reproductive division of labor with a single breeding female, queen (see Figure). Recent work from our group identified a critical role for vocal communication in the organization and maintenance of naked mole-rat social groups. Using machine learning techniques we demonstrated that one vocalization type, the soft chirp, encodes information about individual identity and colony membership. Colony specific vocal dialects can be learned early in life – pups that were cross-fostered acquired the dialect of their adoptive colonies. We also demonstrate that vocal dialects are influenced in part by the presence of the queen. Here, I summarize these findings and highlight our current work investigating how social and vocal complexity evolved in parallel in closely related species throughout the Bathyergidae family of African mole-rats.

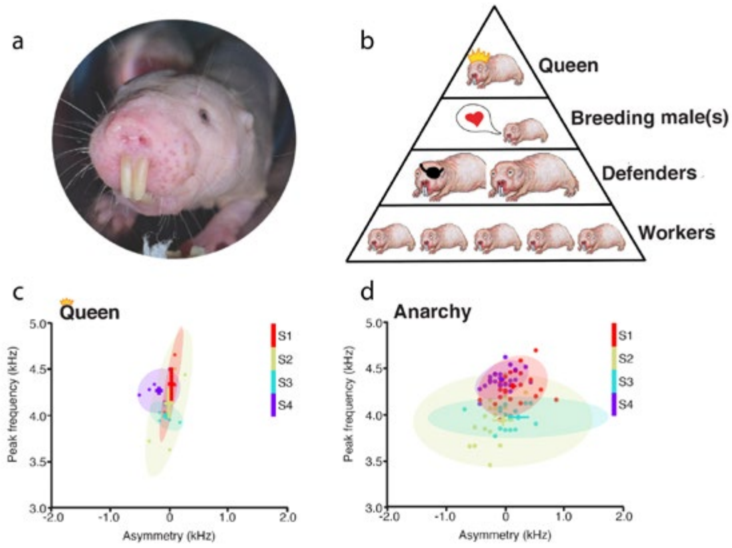


Figure Legend: (a) Naked mole-rats are subterranean hairless rodents. (b) Schematic of the social structure of naked mole-rat colonies. Naked mole-rats are highly hierarchical with a single breeding female, queen. (c-d) The vocal dialect of a colony becomes increasingly variable when the Queen is removed from the colony. Here the vocal variance of four workers (subordinates, S1-S4) are plotted during periods with a Queen or during Anarchy (no Queen). Two sound features of one vocalization type are plotted here, (peak frequency vs. asymmetry). Modified from Barker et al., 2021a. Naked mole-rat illustration: R. Hodge

Glossary

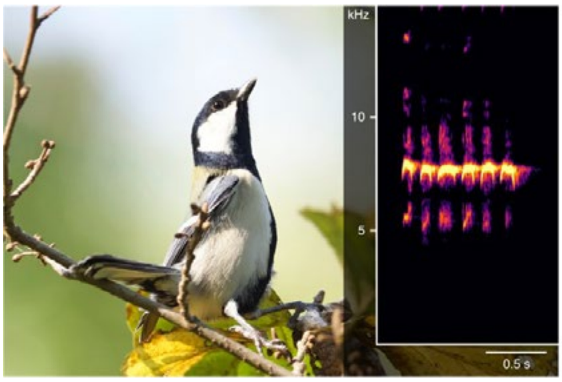
Machine learning: a type of artificial intelligence which employs computer algorithms that can “learn” to improve performance with new data but without explicit programming.

Eusociality: an extreme form of social organization characterized by a reproductive division of labor, shared care of young and multigenerational living. First described in social insects (e.g. bees, wasps, and ants).

Animal linguistics: Exploring elements of language in non-human species

Toshitaka Suzuki, Research Center for Advanced Science and Technology, The University of Tokyo

How does language evolve? Although different researchers may define language differently, uncovering the evolution of complex communication systems, such as human language, is a major challenge for science. One promising approach is to focus on the individual cognitive capabilities required for human language and to seek their origins and similarities in non-human animals. However, field studies to identify linguistic capabilities in wild animals have only just begun and its experimental paradigm remains to be developed. Here, I introduce my 17-years field studies exploring linguistic capabilities in a wild bird species, the Japanese tit (Parus minor). This small bird species uses many different call types in a variety of contexts, such as predator encounters or social interactions, and often combines multiple call types into larger sequences. Field experiments have revealed that Japanese tits use these calls to refer to external objects (specific predator types) and to convey compositional messages (two-word phrases). Moreover, novel experimental paradigms have revealed that receiver tits have evolved cognitive capabilities such as the retrieval of mental images and use of syntactic ordering rules. These findings indicate that several linguistic capabilities, such as referential signaling and compositional syntax, once considered to be unique to humans, have evolved in birds. I introduce some novel paradigms for investigating linguistic capabilities in wild animals and propose the methods and goals of a novel scientific discipline, animal linguistics.



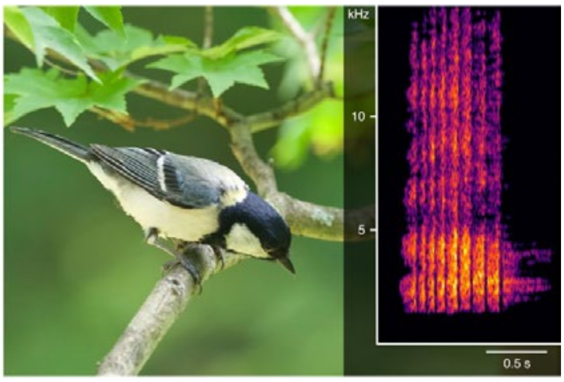


Figure 1. Japanese tits look up to the sky when hearing "hawk" alarm calls (left), whereas they look down on the ground when hearing "snake" alarm calls (right).

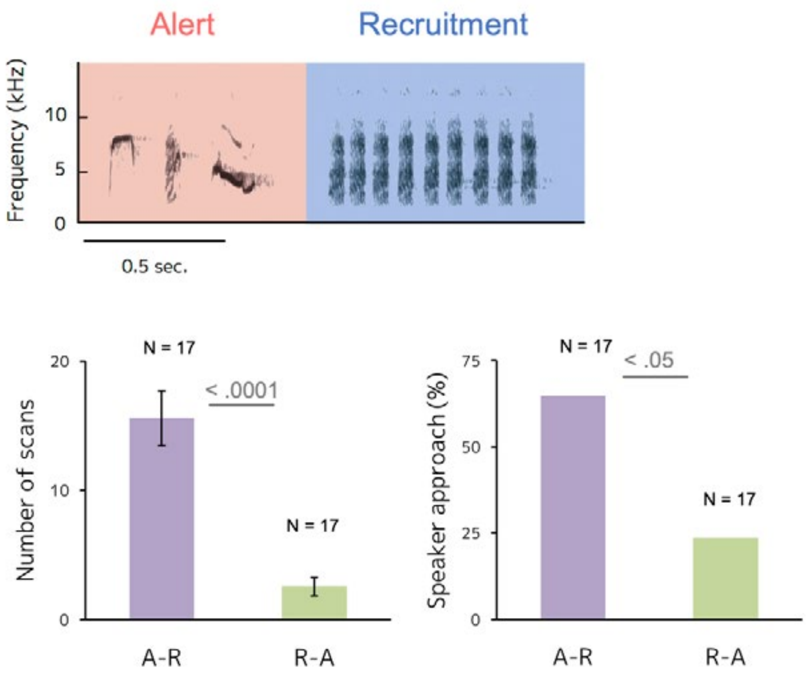


Figure 2. Japanese tits combine alert and recruitment calls into sequences when attracting others to mobbing of a predator (top). Playback experiments showed that Japanese tits reduce their response (both scanning and approaching) if the call order is artificially reversed (bottom), suggesting that these birds use an ordering rule to decode call sequences.

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Glossary

Referential signaling: The ability to communicate about external referents using specific signals, such as predator-specific alarm calls.

Compositional syntax: The ability to combine two meaning-bearing units into sequences that convey compositional information

Introduction to the Session: Environmental Humanities: A Perspective from Commons' Studies

Mihoko Wakamatsu, Tokyo University of Marine Science and Technology

A commons' dilemma is a situation where a group of individuals jointly use a resource, and an individual's rational decision to utilize the resource is sub-optimal from the perspective of the group. This often leads to overexploitation of the resource or underinvestment in its management as introduced by Hardin's Tragedy of the Commons or Olson's Logic of Collective Action. Direct regulation, or so-called command-and-control, has been a standard management tool for regulators in balancing the conservation of resources and achieving economic efficiency of resource use. However, direct regulations are often ineffective in achieving these goals partly because it requires regulators to have an extensive knowledge on a resource and its users' activities. In economics, incentive-based mechanisms such as environmental taxes and emissions trading are considered more efficient. However, such policies are not equally effective in all circumstances. Co-management has been recognized as an important scheme in successfully governing common-pool resources. Contrary to the theory, empirical research has found many long-lasting self-governing communities through extensive case studies. These studies have identified the variables that are considered to be relevant to sustainable resource use and have been summarized as enabling conditions. Examples include small group size and having a good leader in the community. However, these conditions consist of the studies with only successful cases, and no comparison is made with appropriate controls. It is also ambiguous how they are related and what path leads to success. Future studies require the research design that can scientifically verify causal relationship.

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Keywords

Bioeconomy, Neo-Industrialization, Sustainable Development, Public Policy, Brazil

Food, Water and the Climate Crisis: The Micropolitics of Sustainability in Cape Town, South Africa

Katharina Gröne, Wuppertal Institute for Climate, Environment, Energy

In recent years, climate change has induced intensified droughts and shortages of water supply in Cape Town, South Africa. This being a thread to millions of people in itself, it is not the only worrisome event that looms on the horizon. Climate change, biodiversity loss, extreme weather events and unprecedented urban growth intensify resource depletion and food security challenges (will) affect Cape Town's population. All of these challenges represent individual but intertwined strands of the so-called "wicked problems" (Rittel & Webber 1973) of our times. Also referred to as multiple crises, they entangle the global with the local and vice versa. Global institutions claim that they need to be addressed in global, supranational or transboundary partnerships, i.e. through the achievement of the UN's 17 SDGs in joint effort. At the same time, human rights, the access to and the distribution of resources as well as restorative, climate and resource justice are often negotiated locally. This presentation thus situates sustainability in local practices by taking urban agriculture in Cape Town, South Africa as a basis to discuss the micropolitics of inequality and the local power asymmetries in social-ecological endeavours. An analysis of the communicative level of small-scale urban agriculture shows that it is often much more than a subsistence practice or the organisation of a neighbourhood garden. Instead, as the case of the Philippi Horticultural Area Food and Farming Campaign (PHA-FFC) shows, it is also Cape Town's small-scale farmers' practice of resistance against racism and classicism in the social organisation of the city. The PHA-FFC's local and situated negotiation of sustainability boils down to a struggle against discriminatory land-use decisions which affect the food and water security of lower-income households and perpetuate colonial continuities as well as distributive injustices. In the local resistance against the ongoing disenfranchisement of the already marginalised group of black and indigenous small-scale farmers and in their struggle for climate, resource and restorative justice they make use of symbolic codes that question the authority of dominant global institutions in tackling the effects of climate change. Instead, the PHA-FFC links its resistance back to the international small-scale farmers' association La Via Campesina, which engages in struggles about food and seed sovereignty on a global level.

Climate Justice through Indigenous Land Rights

Jessica Hernandez, Landesa

Sea levels are rising, glaciers are melting, and weather patterns are becoming increasingly unpredictable and extreme. These changes are all linked to climate change, which is caused by human activities such as burning fossil fuels, deforestation, etc. Unfortunately, climate change is already having a devastating impact on Indigenous Peoples, animals, and the planet, particularly in the Global South.

In order to build equity and mitigate climate change, Indigenous Peoples from Global South need to be championed in their fight for land rights. Indigenous Peoples have a deep connection to the land and the knowledge (science) to use it sustainably. They are the stewards of the land and should be respected and supported in their efforts to protect it. Climate change can only be effectively addressed when Indigenous Peoples are at the forefront of global climate justice movement.

As part of her research, Dr. Hernandez seeks to develop land-based solutions to build climate resilience and ensure a secure future for Indigenous Peoples and the planet. She works with local communities to identify sustainable, equitable, and culturally appropriate environmental strategies to mitigate and adapt to climate change. Through her work, she advocates for Indigenous land rights to be elevated in global frameworks and sectoral norms, integrated into national policies, and incorporated into local initiatives. In her view, Indigenous land rights should be respected and protected, and governments should prioritize addressing legal gaps that prevent Indigenous people from having access to their lands.

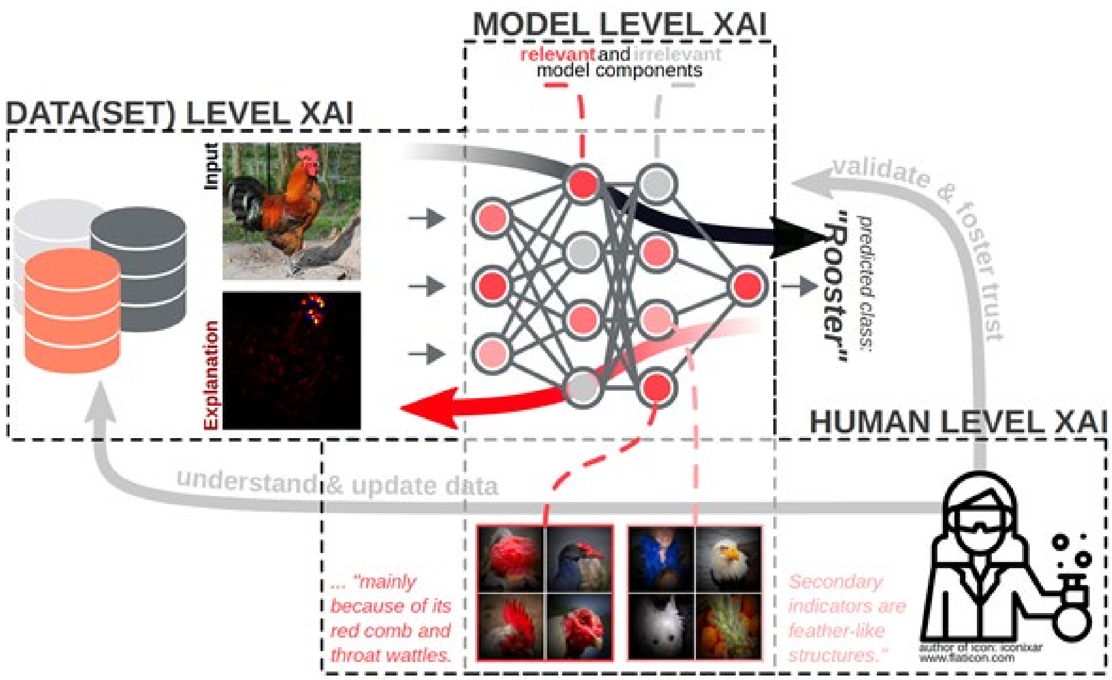
Introduction to the Session: Explainable and Robust Machine Learning

Wojciech Samek, Technical University of Berlin and Fraunhofer Heinrich Hertz Institute

Explainable AI (XAI) has emerged as a critical research field, addressing the need for transparency in highly complex and opaque machine learning (ML) models. This talk aims to introduce the concepts, methods, and recent developments in the field of explainable AI, revolutionizing our ability to understand and interpret previously enigmatic models, such as deep neural networks.

By unveiling the rationale behind model predictions, these explanation techniques offer unprecedented insights and enhance our understanding of complex decision-making processes. Concrete examples will be provided to demonstrate the efficacy of explanation techniques in challenging domains like medical diagnosis and pollution forecasting, showcasing the potential for improved interpretability and trust in AI systems.

A special emphasis will be placed on a novel class of explainable AI techniques known as global-local explanations. These approaches offer a unique perspective by explaining individual predictions in terms of localized and human-understandable concepts *(Human Level).* By dissecting the model's representation *(Model Level)* from the reasoning process on individual input samples *(Data Level),* global-local explanations provide deep insights into the underlying mechanisms and contribute to a more comprehensive understanding of model behavior.



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Furthermore, the talk will delve into recent endeavors within the XAI community that go beyond mere explanation of model behavior. These efforts focus on using explanations to guide model improvement, systematically identifying and addressing undesirable prediction strategies that are misaligned with human intuition. By integrating explanations into the fine-tuning process, biases and spurious correlations in training data can be mitigated, resulting in models that are more robust, fair, and aligned with societal values.

Glossary

Local XAI methods focus on explaining individual predictions made by the ML model. Local XAI techniques often highlight the most relevant features or input components that contributed to the prediction, enabling users to gain insights into the model's reasoning at a local level. For instance, in case of image classification these so-called attribution maps will highlight the pixels and regions in the input image, which are most relevant for the classification.

Global XAI methods focus on explaining the overall behavior and characteristics of the ML model. They aim to provide a comprehensive understanding of how the model functions across the entire dataset and uncover patterns, relationships, and dependencies within the model, shedding light on the model's internal representation and decision-making rules.

Global-local XAI methods aim to capture both the broader patterns and trends exhibited by the model across the entire dataset or domain (global perspective), as well as the specific factors and features influencing individual predictions (local perspective). By leveraging both global and local explanations, global-local XAI strives to offer a more nuanced and complete understanding of the model's decision-making process.

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On Multiplicity of Explanation

Satoshi Hara, Osaka University

Several methods for explaining machine learning models' decisions are developed aiming at overcoming their black-box nature. For instance, if a medical diagnosis model could present an explanation such as “the patient's condition suggests a certain disease”, both the doctor and patient could assess the validity of the diagnosis and decide whether or not to trust it.

In this talk, I will introduce the concept of “multiplicity of explanations” and the challenges it poses. Generally, even when observing the same phenomena, our decisions and explanations may vary from person to person. For example, medical diagnoses and their explanations can vary among doctors. This is due to the difference in each individual's process of thinking and background knowledge. In the context of model explanation, this fact implies that there could be multiple ways to explain the same decision for the same data by the same model. The “multiplicity of explanations” is a difficult concept to handle in machine learning. Many machine learning models output a unique solution through deterministic calculations. That is, one can interpret that the model has implemented only one of the numerous possible “explanations”.

How can we deal with “multiplicity of explanations” in machine learning? One such solution is to enumerate multiple models that can explain the data almost equally well. Each of the multiple models obtained in this way implements a different “explanation”. The studies on “multiplicity of explanations” have also shed light on its negative aspects. With multiple possible explanations, one can choose and provide the “explanation” that is most convenient for them. It is reported that one can generate a fake “explanation” as if a model is making a gender-fair decision, even if a model is actually biased towards gender.

Background Review Article

Leo Breiman, Statistical Modeling: The Two Cultures, Statistical Science, 16 (3):199-215, 2001.

Robust Machine Learning under Distribution Shifts

Han Zhao, University of Illinois Urbana-Champaign

The recent success of machine learning has been largely driven by the availability of large-scale labeled data and models. However, in many real-world applications, the training data may not be representative of the test data, which leads to distribution shifts, causing the trained models to perform poorly when deployed. In this talk, I will present our recent work on understanding and improving the generalization of machine learning models under distribution shifts, including domain adaptation and domain generalization. In domain adaptation, we assume that the training and test data are drawn from different distributions, and the goal is to learn a model that performs well on the test data. In domain generalization, we assume that the training data are drawn from multiple training distributions, and the goal is to learn a model that performs well on unseen test distributions. I will first introduce modern learning algorithms for robust generalization under distribution shifts, and then present my recent work on analyzing and understanding the fundamental limits of these algorithms. Finally, I will focus on designing learning algorithms to escape the existing tradeoff and to generalize under certain distribution shifts with provable guarantees.

Introduction to the Session: Towards global "cloud-resolving" simulation of Weather and Climate

Tomoki Miyakawa, The University of Tokyo

Clouds. Perhaps the most familiar component of weather and climate to the people. They are also the largest source of uncertainty in the global weather/climate system. In traditional numerical models for global simulations, typically with horizontal grid spacing of 50 – 500 km, clouds have been "parameterized" as a simplified function of the grid-scale temperature and humidity profiles. Aided by the recent remarkable improvement of supercomputers, several research groups around the world are developing a new generation of global numerical models, which are designed for being used with horizontal grid spacing of less than 5 km and have the capability to simulate large convective clouds explicitly from fluid-dynamics based integration, without parameterizing them. These advanced models have reached a level of maturity where they can be evaluated and tested in inter-comparison projects such as the "DYAMOND initiative" [1] which now involves 14 participating models. Rich with highly detailed structure of the atmosphere, they have the potential to provide quantum leaps to seasonal predictions of high-impact weathers (e.g., Typhoons, hazardous rain events, droughts, etc.), and to climate projections. These models also serve as powerful tools for deeper understandings of the weather/climate system. For example, the coupling between the atmosphere and ocean/land, interactions between multiple temporal/spatial scales, interaction between the troposphere and stratosphere through cloud-generated atmospheric gravity waves, genesis and development of tropical cyclones, some of which will be further described in detail by Dr. Claudia Stephan and Dr. Falko Judt in their talks.

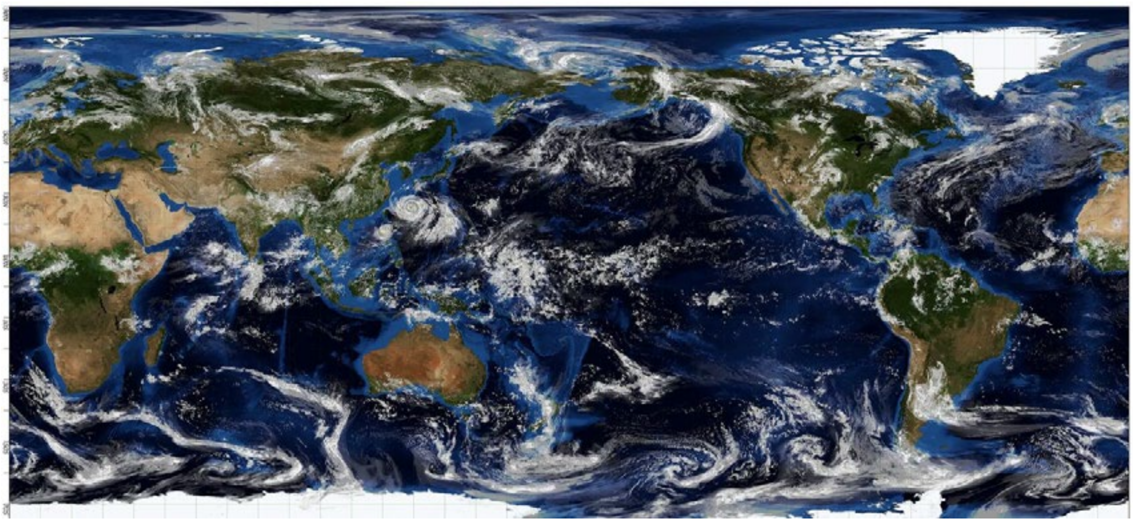

Figure: A snapshot of clouds from the first sub-km grid spacing global simulation [2].

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Background Review Article

Stevens, B., Satoh, M., Auger, L., Biercamp, J., Bretherton, C., Chen, X., Duben, P., Judt, F., Khairoutdinov, M., Klocke, D., Kodama, C., Kornblueh, L., Lin, S.-L., Putman, W., Shibuya, R., Neumann, P., Rober, N., Vannier, B., Vidale, P.-L., Wedi, N., Zhou, L.. 2019: DYAMOND: The DYnamics of the Atmospheric general circulation Modeled On Non-hydrostatic Domains. Progress in Earth and Planetary Science, 6, 61, www.doi.org/10.1186/s40645-019-0304-z.

Improving Tropical Weather and Climate Predictions with Global Cloud-resolving Models

Falko Judt, National Center for Atmospheric Research

Current-generation weather and climate models have long struggled to accurately simulate the intricate dynamics of the tropical atmosphere, resulting in poor forecasts compared to extratropical regions. In particular, current-generation models have difficulty capturing the extreme winds of tropical cyclones and fail to account for variations in tropical rainfall. However, a breakthrough has emerged in the form of global cloud-resolving models, a new class of numerical weather and climate models that leverage the power of the latest supercomputers. These models offer an exciting opportunity to overcome these limitations and improve tropical weather and climate prediction while deepening our understanding of these phenomena.

Employing a “resolution ensemble” of a state-of-the-art numerical weather/climate model, we have demonstrated the value of global cloud-resolving models. As expected, lower resolution versions struggle to accurately simulate tropical weather phenomena, while the high-resolution (“cloud-resolving”) model effectively captures tropical cyclone intensity, and the variations in rainfall caused by tropical weather phenomena. The key distinction lies in cloud-resolving models’ ability to resolve fine-scale features and interactions between clouds and circulations that are crucial to tropical weather.

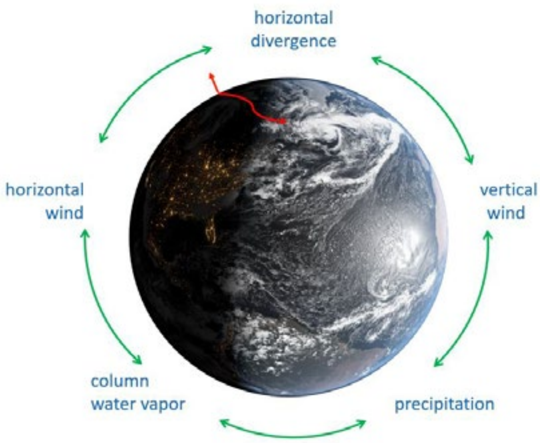
The utilization of global convection-permitting models holds great promise for improving simulations of tropical weather and climate phenomena. However, it is important to acknowledge the associated limitations. The computational costs involved are substantial and require access to high-performance computing resources. Furthermore, variations may exist among different global convection-permitting models, highlighting the need for further investigation and validation to fully unlock their potential and address any biases that may arise.

In conclusion, global cloud-resolving models hold great promise for improving simulations of tropical weather and to effectively anticipate and mitigate the impacts of tropical weather events on vulnerable regions worldwide. The ongoing advancements in global convection-permitting models offer exciting prospects for the future of tropical weather prediction and climate studies. By addressing the computational challenges, conducting further research, and validating the models, we can maximize their potential and ensure their reliable application.

The coupling of motion and moisture fields from cloud scales to global scales

Claudia Stephan, Max Planck Institute for Meteorology

We are well able to observe clouds, but understanding the connection between moist processes and motion fields has been a long-standing goal, as the three-dimensional wind field is difficult to observe directly. Global kilometer-scale modeling makes the link between small-scale convection and the large-scale circulation a new frontier, and this frontier is the topic of my talk. The complex, multiscale nature of atmospheric variability, in both space and time, has always presented a challenge for theoretical understanding. Clouds are undeniably relevant for climate themselves. But in addition, like a stone thrown into a pond, the energy release from condensation generates internal atmospheric waves, which in turn drive global circulation patterns. I will explain why convection on short spatial scales has first-order effects on larger scales and mean aspects of climate. Moreover, as it turns out, there exist feedbacks in the opposite direction as well: atmospheric waves and mean flows shape the moisture and vertical motion fields, and these define the statistical properties of convection. Particularly in the tropics, convection and atmospheric circulation are inextricably linked. I will present a summary of our newly gained understanding of how spatial spectra of horizontal motion, vertical motion, and precipitation are physically linked. We gained this understanding thanks to the new species of models, which let us overcome a notorious 'road block' of numerical modeling, as we can now explicitly model wave sources and wave motions including their feedback on their sources based on physical equations.



Kilometer scale models

- resolve vertical energy and momentum transport, hence e xplicit scale interactions
- have realistic orography and transient precipitation dynamics, hence wave sources
- approach the scales we observe, hence let us test physical hypotheses

Further reading:

These general articles can probably be understood by scientists who do not work in atmospheric science.

The philosophy of why we want kilometer-scale models

Slingo et al., 2022: Ambitious partnership needed for reliable climate prediction
https://www-nature-com.e-bis.mpimet.mpg.de/articles/s41558-022-01384-8

Palmer and Stevens, 2019: The scientific challenge of understanding and estimating climate change
https://europepmc.org/backend/ptpmcrender.fcgi?accid=PMC6900733&blobtype=pdf

Computational aspects

Schär et al., 2020: Kilometer-Scale Climate Models: Prospects and Challenges
https://doi.org/10.1175/BAMS-D-18-0167.1

New models require new analysis strategies

Stephan et al., 2020: Waves and coherent flows in the tropical atmosphere: new opportunities, old *challenges*
https://rmets.onlinelibrary.wiley.com/doi/full/10.1002/qj.4109

If you would like to dive deep into the details, i.e. theory, have a look at my publication list:
mpimet.mpg.de/fileadmin/portfolios/36/publications.pdf

Introduction to the Session: Quantum Science and Technology

Uri Vool, Max Planck Institute for Chemical Physics of Solids

Though the world we live in appears to be made of solid objects with fixed position, velocity, etc., when we look closely these solids turn out to all be made of fuzzy probability waves. This remarkable realization, during the first decades of the 20th century, revolutionized our fundamental understanding of the world and let to various technological innovations. Commonly used devices such as computer chips, LEDs, lasers, and MRI machines are entirely based on quantum effects. However, in materials made up of many particles, quantum effects are typically averaged out to give rise to our classical world. While the devices mentioned above make use of quantum effects, their probability waves are smeared out. Macroscopic objects which retain their probability wave, such as the famous "Schrödinger's cat" which is both dead and alive, were until recently seen as mere thought experiments that can never be implemented.

However, since the 1980s improvements in material quality and device control have given us increasing ability to create true Schrödinger cats in various physical platforms, with system size and control improving every year. This "second quantum revolution" has created excitement for a potential new class of devices which take full advantage of the strange quantum waves. Though the field is still very new, it promises technological breakthroughs in various fields, such as secure communication, sensitive measurements, and fast computation.

In this talk, we will discuss these new quantum systems and how quantum coherence can be used for technological advantage. We will also discuss the various physical implementations of quantum systems, from isolated atoms, through "artificial atoms" in solid state systems and eventually to complex quantum materials.

Molecular Quantum Information Science with Electron Spins

Ryan G. Hadt, California Institute of Technology

We are experiencing a second quantum revolution. Subsequent to the development of quantum mechanics – the first quantum revolution – current research in molecular Quantum Information Science (QIS) seeks to develop new quantum-enabled technologies, ideally operating under ambient conditions, for computation, communication, and sensing by controlling quantum phenomena such as superposition, entanglement, and coherence. Molecules with unpaired electron spins constitute a platform for the physical implemention of a quantum bit (qubit), the fundamental unit of quantum information. Quantum devices based on molecules therefore afford unique potential in miniaturization, spatial localization, and tunability through synthetic chemistry. Coherent quantum states can be generated by interacting electron spins with electromagnetic radiation (e.g., microwaves and/or visible light). However, these coherent states are inherently out-of-equilibrium and will return to equilibrium by interacting with their surrounding environment, leading to spin relaxation and, ultimately, the loss of quantum information. While the electron spin relaxation processes important for applications in QIS have been rationalized on the basis of the Debye model, the assumptions behind this model are incompatible with the structure of molecular materials and, thus, this approach does not yield meaningful insights or predictions for slowly-relaxing, highly coherent molecules. A new approach rooted in molecular structure is therefore required to fully understand high temperature decoherence mechanisms. Our lack of current understanding stems from a dearth of experimental studies and approaches aimed at probing the key chemical bonding contributions to spin relaxation mechanisms. To address these issues, our research has employed and developed new lines of spectroscopic inquiry to quantitatively evaluate the critical interactions that control high temperature quantum coherence in molecular systems. This talk will illustrate how we have learned to define and control the interactions between electron spins and dynamic molecular structure to achieve long-lived coherent states and will describe the development of ligand field electron spin dynamics, a new molecular paradigm with which to understand how electron spin relaxation leads to the loss of quantum information. Our combined experimental and theoretical analyses provide spin relaxation structure-function relationships and elucidate the critical chemical bonding, symmetry, and ligand field excited state coupling factors enabling room temperature coherence.

Solving chemistry problems on a quantum computer

Kenji Sugisaki, Keio University

Quantum computers are powerful computing devices that have the potential to solve some specific problems exponentially faster than the traditional computers. Quantum computers are computers that operate according to quantum mechanical principles, and they can use quantum superpositions and quantum entanglements as their computational resources. Among the diverse topics in the field of quantum science and technology, solving the electronic structure of atoms and molecules, known as a quantum chemical calculation, has been considered as one of the most promising applications of quantum computers. Quantum chemical calculations can deal with molecules that are too unstable to isolate experimentally and that have never been synthesized. Thus, accurate quantum chemical calculations can open the door to the theoretical design of new materials and drugs.

In the conventional quantum chemical calculations, we calculate the total energies of molecules using the atomic coordinates as the input. By comparing the total energies of molecules with different molecular structures, we can discuss, for example, how stable the molecules under study are, what types of chemical reactions they undergo, and how much energies they need to occur chemical reactions. In this context, energy differences are much more important than the total energies themselves for discussing chemical phenomena. Because quantum computers can use quantum superposition states as their computational resources, they are able to directly compute the energy difference between two different electronic states or geometries, without inspecting total energies of the individual electronic states. In this talk I will introduce a quantum phase difference estimation algorithm as the general quantum algorithm for the direct calculation of energy differences on a quantum computer[1-4].

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Glossary

Quantum superposition: Traditional quantum computers use a “bit” as the fundamental unit of information. A bit can represent either a 0 or a 1. In contrast, quantum computers use a “qubit” to store and process information. Unlike bits, qubits can exist in a superposition state which is an arbitrary linear combination of the $|0\rangle$ and $|1\rangle$ states.

Quantum entanglement: Since qubits can be in quantum superposition, the quantum states of multiple qubits can be “entangled”. When the quantum states are entangled, the measurement of one qubit affects the quantum state of other qubits.

Introduction to the Session: Rewriting the History of our Universe with the James Webb Space Telescope

Katherine E. Whitaker, University of Massachusetts Amherst

The first year of observations from the James Webb Space Telescope have revolutionized our understanding of the Universe. Webb is bringing us closer to a qualitatively new view of Earth-like worlds outside of our own Solar System, with the capabilities to search for the chemical fingerprints of life and already confirmation of an extrasolar astroid belt and water within an exo-atmosphere. Zooming out to larger scales, Webb has revealed stellar nurseries within our own Milky Way in spectacular new detail. And one of the most fundamental paradigm shifts has come with our understanding of the most distant galaxies, looking >13 billion years into the past. The first galaxies seem to be forming earlier and more rapidly than previously thought, defying predictions from our best theoretical models. There is also a surprising population of actively accreting supermassive black holes in these distant galaxies.

Webb is a 6.5 meter telescope that is sensitive to infrared light, giving us a revolutionary view of the ‘Red Universe’. The telescope was launched on December 25, 2021 and traveled 1 million miles from Earth while unfolding itself and a tennis-court-sized sunshield on its way to its current home, a semi-stable orbit at the Earth-Sun second legrange point. To operate at infrared wavelengths, the sunshield allows the telescope to cool down below -370°F, with the Sun heating up the ‘hot side’ as high as 185°F. If that was not enough of a technological feat, this first year of data starting from July 2022 onward has unambiguously demonstrated that this telescope is performing even greater than expectations.

In this talk, I will provide you with an introduction to the capabilities of NASA/ESA’s new flagship mission and highlight a few of the most exciting and revolutionary results in the literature to date. Among these is the story of distinguishing the most distant galaxies from galaxies enshrouded in thick veils of dust, while also teasing out hidden supermassive black holes at their hearts from the mix. With every new mission comes important lessons, and there have been no shortage along the way to these ground-breaking discoveries. The talk will end with a look to the future and all of the exciting new discoveries just on the horizon from nearby exoplanets to the furthest reaches of our Universe.

Exoplanet Science in the era of JWST

Yui Kawashima, Japan Aerospace Exploration Agency

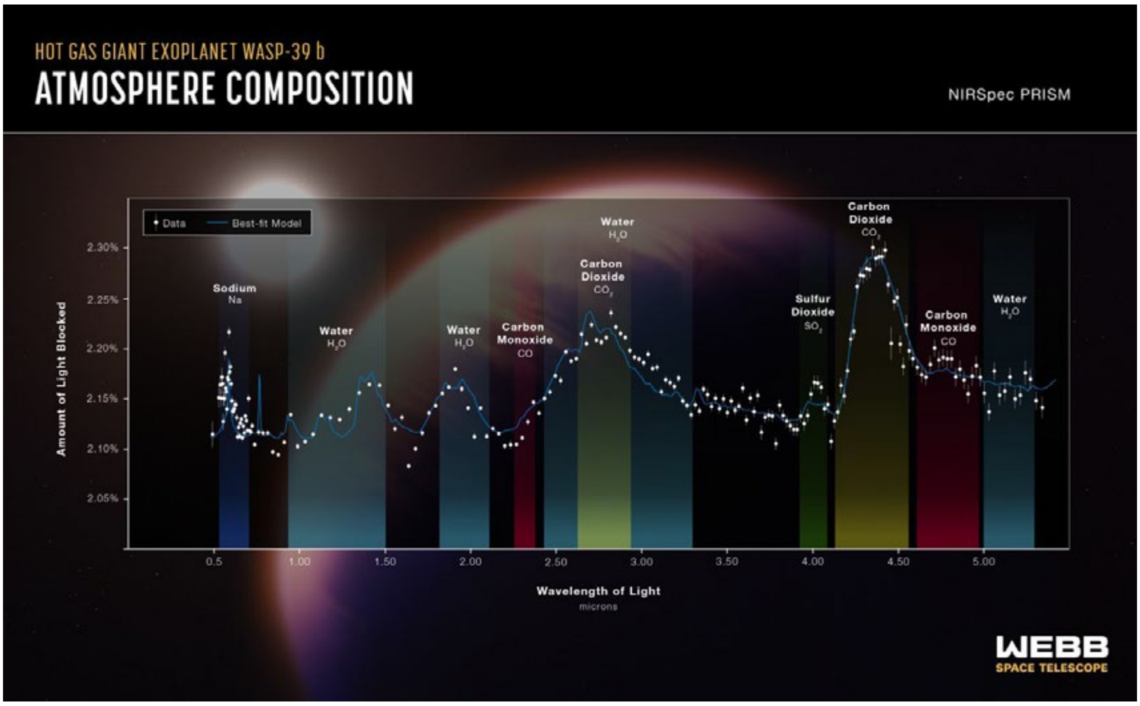

Figure 1: The atmospheric spectrum of a hot gas giant exoplanet WASP-39b observed by the James Webb Space Telescope (https://esawebb.org/images/weic2221f/). The spectrum shows the absorption features of various chemical species.

Exoplanets, planets orbiting stars other than the Sun, were first discovered in 1995. Since then, the detection of more than 5,000 exoplanets has been reported. Those discoveries include planetary systems significantly different from our solar system, such as the system with a Jupiter-sized planet in orbit closer than that of Mercury in our solar system [1] and the system with seven Earth-like planets [2]. To reveal the origin of such diversity of planets, namely their formation and evolution processes, and assess their habitability, it is essential to understand their atmospheres. By performing the spectroscopy of planets with the use of telescopes, we can acquire information on the composition and structure of the atmospheres. However, due to the precision and wavelength coverage of the existing telescopes, the planets we could observe and the chemical species we could search for were limited.

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At the end of 2021, NASA's new flagship telescope, the James Webb Space Telescope (JWST), was successfully launched, which has dramatically changed the situation. Thanks to the excellent precision and broad wavelength coverage of JWST, we can now precisely measure the abundance of various chemical species that are present in the atmosphere for a number of exoplanets, which is crucial to reliably explore the formation/evolution processes and habitability of the planets. In this talk, I will give an overview of the recent results regarding the atmospheric characterization of exoplanets by JWST (e.g., [3], [4], [5]), including the first solid detection of a photochemical product SO2 in exoplanet atmospheres [6], together with future perspectives.

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Glossary

Exoplanet: A planet orbiting a star other than the Sun. The first exoplanet was found in 1995.

Transit observation: When a planet passes in front of the star as seen from the Earth, the stellar brightness slightly decreases. Transit observation is the method to discover the planet by detecting that slight decrease in the stellar brightness.

Transit depth: The amount of the decrease in the stellar brightness during a transit event. Since transit depth is proportional to the ratio of the stellar area the planet covers, one can infer planetary radius from the measurement of the transit depth.

Transmission spectrum: Transit depth as a function of the wavelength. Since the amount of extinction by molecules and clouds in the planetary atmosphere differs by the observational wavelength, one can infer atmospheric composition from the observation of the transmission spectrum.

Background Review Article

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Exploring the Dark Cosmos through Gravitational Lensing and the James Webb Space Telescope

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The enormous sea of stars that fills a clear night sky and all the Earthly matter that we see account for only 5% of the energy budget of the Universe. About 25% is in the form of "dark matter" and the remaining 70% is the so-called "dark energy", both of which are nature's great puzzles. Dark matter is difficult to detect because it does not emit light, but it interacts gravitationally with the luminous matter that are visible. Such interactions provide a way to detect and study dark matter. Dark energy is accelerating the expansion of our Universe, but the nature of dark energy remains elusive.

In this presentation, I will show how gravitational lensing, a spectacular phenomenon where light is bent around massive objects, probes dark matter, dark energy and the cosmic expansion. The James Webb Space Telescope has produced fantastic images and spectra of gravitational lenses in the infrared that allow us to peer deep into space. The attached figure is the first image taken of the galaxy cluster SMACS 0723, showing a cluster of galaxies that acts as a giant gravitational lens, magnifying and lensing distant galaxies behind the cluster into large arcs on the sky. This lensing effect provides a powerful way to study the dark cosmos.

JWST image of SMACS 0723 showing a galaxy cluster that is gravitationally lensing galaxies behind it into arcs. Image credits: NASA, ESA, CSA, STScI.