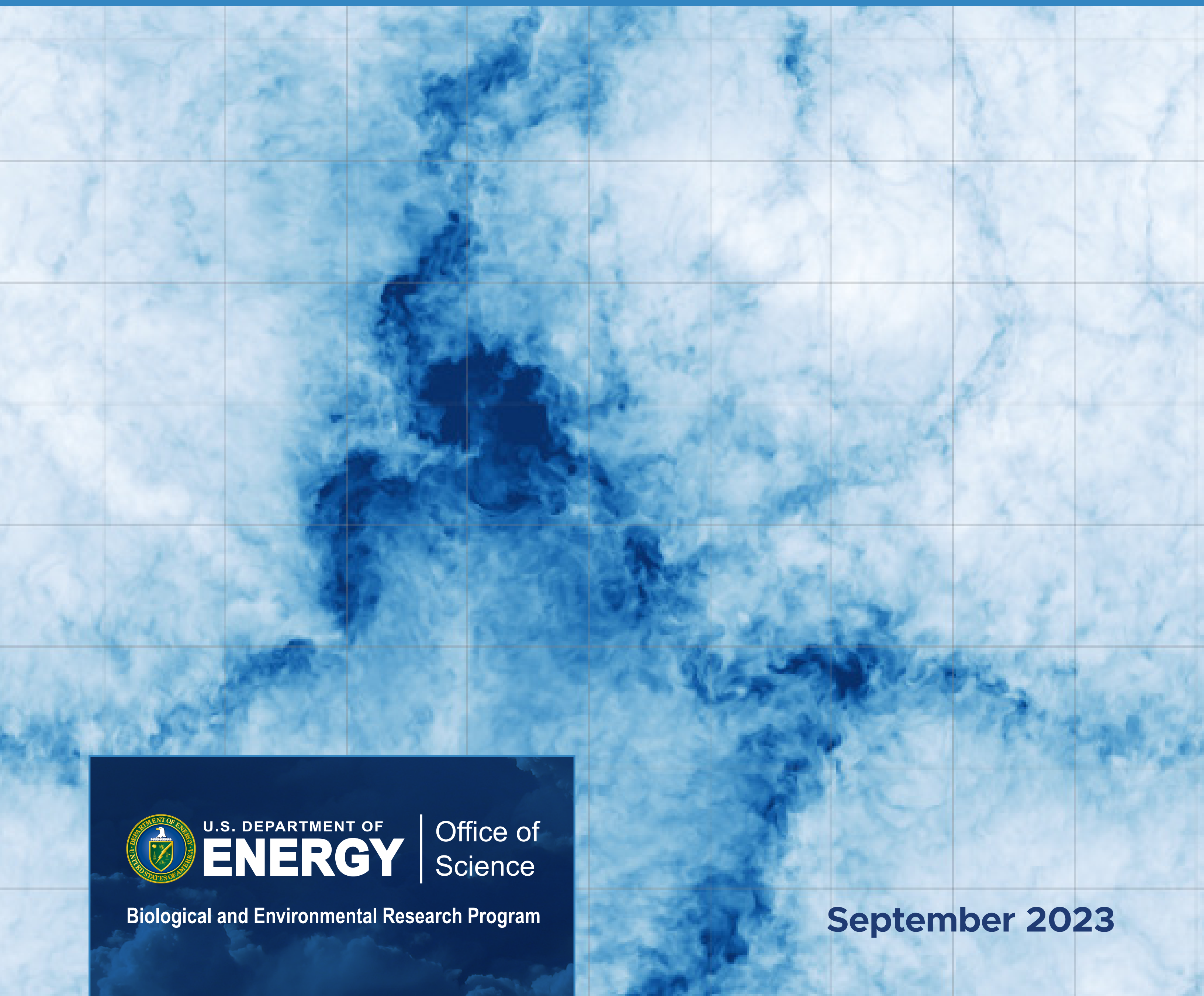
DOE/SC-0212

Department of Energy's Atmospheric System Research (ASR) Program's Workshop on the Future of Atmospheric Large Eddy Simulation (LES)

WORKSHOP REPORT



U.S. DEPARTMENT OF ENERGY | Office of Science

Biological and Environmental Research Program

September 2023

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Cover Image: This image shows the output of a large eddy simulation (LES), roughly illustrating a view of stratocumulus clouds from an aircraft while flying over the ocean.

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EXECUTIVE SUMMARY

Large-eddy simulation (LES) is used as a tool to understand physical processes such as turbulence, aerosols, clouds, precipitation, radiation, the interactions among all these, and their interactions with the underlying surface. Over the next 10 years, LES will drive fundamental progress in open scientific questions in these areas as LES is increasingly used to gain understanding of complex interacting physical processes involving atmospheric turbulence. This growth will be driven both by scientific demand and the expansion of computational resources needed to conduct LES, and the form that the growth takes will largely be determined by how computational resources are leveraged for scientific gain. In particular, we suggest that computational resources are likely to be leveraged in two separate but not necessarily distinct ways. On one hand, growth in computational resources will allow LES to be made more routine, that is, performed more frequently, while on the other hand, the computational expense (measured in total floating point operations) afforded to individual LES will expand dramatically, allowing simulations to increase in both domain size and resolution as well as physical detail.

Current U.S. Department of Energy (DOE) projects such as LES ARM Symbiotic Simulation and Observation Activity (LASSO) are leading the way in conducting routine LES, building large, public databases that are accessible for data science, sensitivity studies, and training for machine learning. LES will also become more routine as it becomes more accessible for individual researchers to address their scientific questions of interest. Scientific questions addressed by LES over the next 10 years are likely to include cloud organization and aggregation; aerosol cloud interactions and atmospheric chemistry (including geo-engineering); urban-scale LES; atmospheric extreme events, ranging from small-scale severe weather to wildfires; and ocean-wave-atmosphere interactions. Further LES-related research will likely grow significantly in areas related to societal impact studies of air quality and extreme weather events, applications to renewable energy forecasting and resource assessment, and aid in decision-making processes.

The growth in the use of LES in atmospheric science research will drive the need for better physical process representations (e.g., cloud-aerosol microphysics, radiation, and atmospheric chemistry) at the scales resolved by LES. To date, many of the process representations used by LES have been taken directly from coarser-resolution models. Promising methods for LES process representations include superdroplet and quadrature methods for microphysics, 3D approaches for radiation, and better representation of chemistry and aerosol processes. At LES resolution, land-atmosphere interactions for complex terrains, land cover/types, biogeochemistry, and plant canopy models are needed as an improvement beyond traditional and widely used Monin-Obuhkov similarity theory.

Further opportunities exist to drive science through synergistic efforts involving LES, real-world observations, and laboratory studies. For instance, there are opportunities for Observational System Simulation Experiments (OSSEs), in which LES can help optimize observational campaign pre-deployment strategies to answer specific scientific questions. Further, observations and laboratory studies can serve particular and distinct roles in validating LES and developing parameterizations for it. Instrument simulators are greatly needed to facilitate apple-to-apple validation of LES against observations and are likely to play an important role in both OSSEs and model validation. It is highly desirable for model validations and machine learning studies to have representative long-term continuous sampling of different weather/climate regimes, especially characterizing spatial heterogeneity. It will be highly useful to develop observationally constrained case libraries, especially for those regimes or processes associated with climate sensitivities. Such libraries should not only have initial and boundary conditions and large-scale forcings to drive models, but also a set of observational diagnostics and statistics to validate models.

Thus far, LES modeling has traditionally been disjoint from efforts involving global Earth system models (ESMs). There are unique opportunities for DOE-supported science to bridge the gap between LES and ESMs. For example, offline coupling of state-of-the-art LES to DOE's Energy Exascale Earth System Model (E3SM) allows the use of LES to study how atmospheric processes change with climate, perform forward-looking renewable energy resource assessment, and predict societal impacts under climate change. Coupling between LES and ESM will require attention to high-temporal-frequency lateral boundary conditions, more detailed land surface data sets, and possibly considerations of data assimilation.

Maximizing use of growing computational resources is requiring LES software to adapt, potentially rapidly, to emergent high-performance computing (HPC) hardware. To this end, atmospheric models are increasingly being written in languages that facilitate hardware portability and/or execution on general-purpose graphical processing units, and away from Fortran, which has been the dominant language of atmospheric models for decades. However, this shift has come with consequences, as there is limited software engineering experience within the atmospheric science community in many of these languages. It would be highly desirable to explore opportunities to ameliorate these consequences by fostering opportunities to nurture software engineering expertise within the atmospheric science community and/or to seek opportunities to achieve hardware portability and performance in models written in languages like Python that have already been widely adopted within the atmospheric science community.

Historically, much LES research can be separated into idealized LES (e.g., with horizontally periodic boundary) and realistic LES (e.g., with lateral boundaries prescribed from larger-scale models). It is important to bridge the gap between the realistic LES and idealized LES communities while acknowledging that both enable fundamental research advances.

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1.0 WORKSHOP BACKGROUND AND OVERVIEW

Large-eddy simulation (LES) is a modeling approach that solves spatially filtered equations of fluid motion and explicitly simulates the scales of turbulence larger than the filter scale. In the atmosphere, given unlimited computing resources, LES could be well applied to resolve turbulence having scales ranging from hundreds of meters to millimeters and time scales ranging from minutes to milliseconds. However, LES is computationally expensive, so that only small domains with a horizontal size of ~10km or less can be simulated in real time. Large-domain LES for deep convective processes, such as convection aggregation or mesoscale convective systems, while highly desired, are very limited by computational resources available. Highly non-linear processes, such as detailed microphysics, chemistry, or radiation, are still parameterized as subgrid-scale processes, in a similar way as in larger-scale models. Because LES provides an explicit representation of three-dimensional turbulence, it has emerged as the modeling tool of choice for simulating atmospheric processes that interact with such turbulence. LES is currently applied to a range of applications with a hierarchy of complexity ranging from simulations of highly idealized boundary layers, to idealized studies of how clouds change with environmental conditions, up to simulations of real cases with detailed representations of cloud microphysics, chemistry, and the land surface. Such studies support DOE's and the Atmospheric System Research (ASR) program's goal "to advance the process-level understanding of the key interactions among aerosols, clouds, precipitation, radiation, dynamics, and thermodynamics, with the ultimate goal of reducing the uncertainty in global and regional Earth system models." Further, as LES explicitly represents many of the processes parameterized in coarser-resolution models, LES serves as a data source for the development and validation of parameterizations for these models.

The use of LES will expand as computational resources continue to grow, enabling the application of LES to simulate a broader range of processes and scales. It is these important roles filled by LES that motivated the creation of *The Department of Energy's Atmospheric System Research (ASR) Program's Workshop on the Future of Atmospheric Large-Eddy Simulation (LES)*, which was held virtually April 25 and 26, 2022, with the purpose of leveraging the expertise of **LES developers, process modelers**, and **observationalists** to identify the current state of the science, the most pressing research challenges, and pathways forward that may prove valuable to progressing the science.

The workshop sought to answer five unifying questions:

1. What are the opportunities for LES-related research for atmospheric aerosol, cloud, and precipitation process studies over the next 5 to 10 years?
2. What physical process representations in LES will limit research progress over the next 10 years?
3. What aspects of current LES implementations will limit research progress over the next 10 years?
4. What kind of observations would be useful in improving and further validating LES?
5. What opportunities exist for improved synergy between observations and LES in studies of the atmosphere, and what are the challenges in doing so?

The workshop consisted of four general sessions, each with a separate area of focus:

1. **History of LES and LES in ASR**–The evolution of LES and its application broadly and specifically in ASR from its inception to today.
2. **Process Science**–Use of LES to advance process science and the interplay between LES and observations.
3. **LES Model Physics**–Representation (parameterization) of physical processes in LES.
4. **LES Development**–Technical/software development for atmospheric LES.

Each focus area featured plenary speakers and a discussion period (moderated by the plenary speakers and a member of the organizing committee) guided to address the five workshop unifying questions. All workshop participants, excluding plenary speakers, were asked to prepare a poster highlighting their LES relevant research as well as to respond explicitly to the unifying questions. The workshop featured poster sessions for each of the four general sessions. Workshop organizers assigned posters to sessions based on poster content. There were no parallel or breakout sessions during the workshop and attendees were encouraged to participate in all sessions.

The general sessions were hosted on Zoom with chat-based discussions hosted on Slack. Poster sessions were hosted on Slack exclusively. Zoom recordings of the general sessions, Slack-based discussions, and posters were the primary source material for this report. The goal of this report is to synthesize the information gathered during the workshop's general and poster sessions to provide a view of valuable LES-related scientific and development endeavors that have the potential to expand the impact of LES in achieving the scientific objectives of DOE and ASR in particular, and the atmospheric sciences in general.

This report includes references to the peer-reviewed literature to provide context and to help identify the state of the art as a means of finding launch points for future work. The appendices provide a list of workshop attendees, the workshop's agenda, and the approach to a highly interactive, online workshop.

2.0 ADDRESSING THE FIVE UNIFYING QUESTIONS

2.1 What Are the Opportunities for LES-Related Research for Atmospheric Aerosol, Cloud, and Precipitation Process Studies over the Next 5 to 10 Years?

Continued advances in and availability of HPC resources are expanding the range of scientific problems to which LES can be applied and are changing the way in which the LES community thinks about research involving LES. The growth of computational resources has had two primary effects. First, the availability of HPC resources has made LES more routine, allowing more frequent and more numerous LES to be performed. This builds on foundations laid by projects like DOE's Atmospheric Radiation Measurement (ARM) user facility's LASSO (Gustafson et al. 2020). Second, the sizes of the largest simulations (in terms of computational expense) that are attainable given HPC resources continue to increase, allowing simulations to have increased domain size, domain resolution, and complexity of physical process representations. We will address these two effects separately.

2.1.1 Routine LES

Routine LES opens many opportunities and makes LES accessible to a larger group of users. The availability of output from routine LES expands both the LES community and the range of applications of LES. Workshop participants noted that the need to obtain HPC resources to perform LES can be a barrier to participation – the availability of routine LES output overcomes this barrier. Another important aspect of making LES accessible is by improving the user friendliness and/or understandability of LES codes, recognizing that when LES non-experts can quickly and confidently set up and run LES and be reasonably sure that they have done so correctly, they are more likely to do it. While this is good practice in model development in general, it is of particular importance when trying to stimulate non-expert users to use the tools independently, and therefore more critical for community codes.

2.1.1.1 Statistical Robustness and Uncertainty Quantification in LES

Routine LES will allow LES to be run in larger numbers (i.e., as ensembles), facilitating uncertainty quantification and statistically robust analysis of LES results, both of which require large numbers of simulations to be performed. Historically, the computational expense of LES has prevented widespread and rigorous uncertainty quantification (e.g., Jansson et al. 2021, Kaul et al. 2022) and sensitivity studies of LES. Uncertainty quantification is critical for making targeted improvements to existing LES models and exposing opportunities for new developments, especially when formal uncertainty propagation is linked with physics-based understanding of the diagnosed uncertainties.

LES uncertainty quantification is essential in justifying the use of LES as a "truth" data set in the context of machine learning or in the use of LES in OSSEs in support of planning observational strategies for field campaigns (Zeng et al. 2020).

2.1.1.2 Integrated Model-Observation-Experiment Paradigm (ModEx)

There is a clear opportunity for routine LES to support the DOE Biological and Environmental Research program's model-experiment (ModEx) approach. It is likely that LES will play a fundamental role as the "Fine-Scale" modeling component in the ModEx workflow depicted in Figure 1 and that LES will be particularly useful in this role in shaping observational strategies (for example, through OSSEs), enhancing spatio-temporally sparse observations to yield fine-scale process understanding, and with observational validation as ground truth to "Intermediate-Scale" and "Large-Scale Models". Further, within the ModEx paradigm, LES may play an important role in an explicitly coupled Fine-Scale–Intermediate-Scale–Large-Scale model hierarchy.

There are also challenges to applying LES to ModEx. An essential element of the ModEx paradigm, as an iterative design process, is rapid model prototyping to accelerate the rate of iteration. In the context of LES, this will require agile and extensible software design strategies as well as development of LES models that can be integrated with rapid turn-around times. Additionally, the iterative nature of ModEx requires LES to be run frequently, which is computationally expensive.

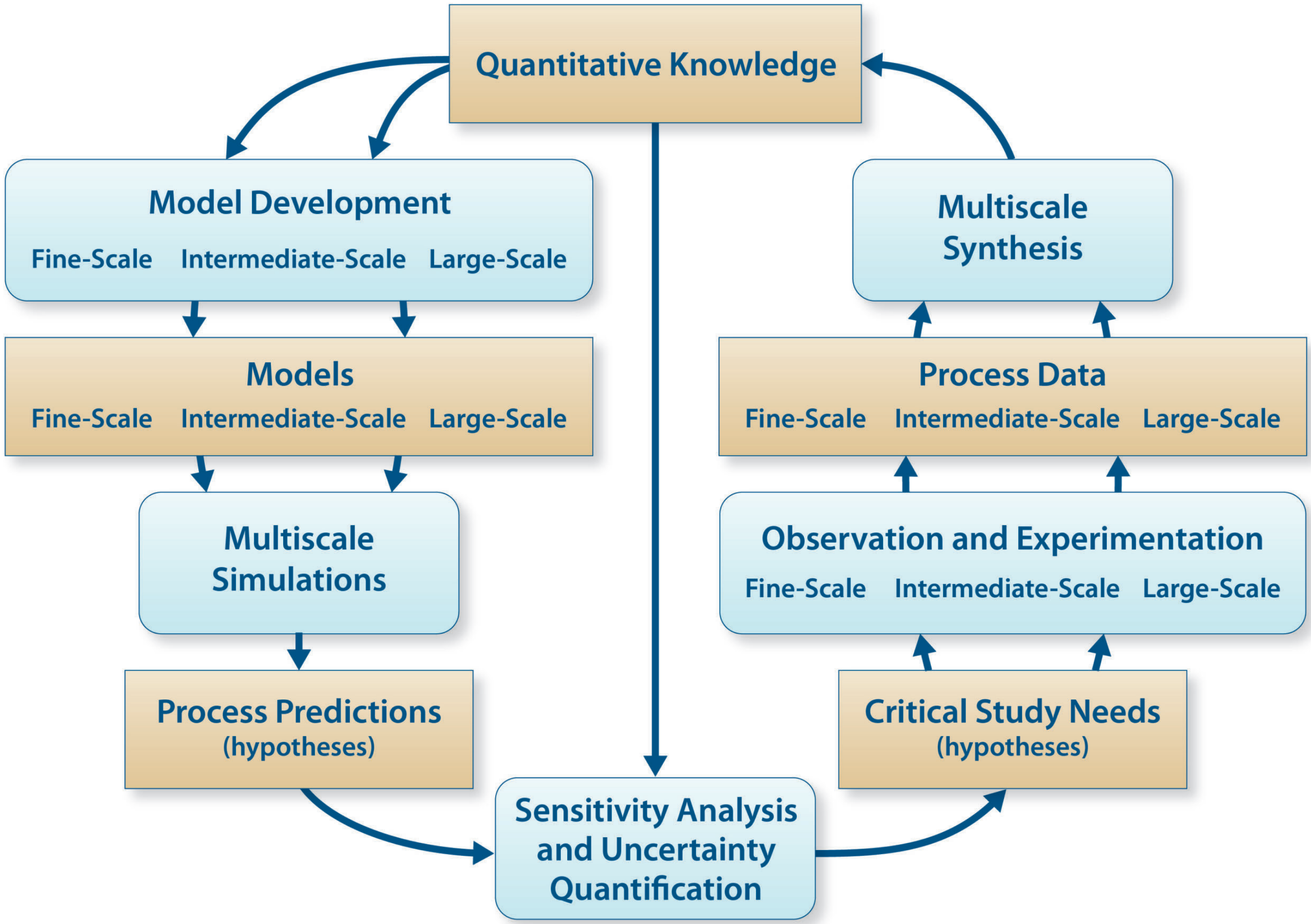

Figure 1. Model-experiment (ModEx) workflow. *Image courtesy of DOE Environmental System Science Program.*

2.1.1.3 Generation of Large Ensemble of LES for Wide-Ranging Conditions

Increasing demands are being placed on LES to provide diverse training data sets to support machine learning approaches. Such approaches can be used to address highly uncertain physical process representations in other models, for example, microphysics-aerosol-turbulence interactions. Routine LES makes generation of these training data sets attainable (e.g., Cheng et al. 2022, Shen et al. 2022). However, the community has not yet determined how best to create training data sets with sufficient diversity to ensure adequate generality of emulators intended for use in climate and numerical weather prediction (NWP) models. At present, this is a challenge due to the complexity of configuring initial conditions and large-scale forcing for LES to simulate a particular atmospheric state. A reasonable goal for the LES community over the next five to ten years is to develop workflows for rapidly prototyping and developing LES that span the wide ranges of conditions necessary to develop diverse and trustworthy training data sets.

2.1.2 Increasing Computational Complexity of LES

With more HPC resources available, more computationally complex problems can now be resolved by LES. Here we define the computational complexity of LES in the computer science sense as the amount of computational resources necessary for execution. Note that greater computational complexity does not imply greater software complexity nor greater complexity of the model's underlying algorithms. Increasing the maximum computational complexity shapes the opportunities for atmospheric aerosol, cloud, and precipitation process studies in several ways.

2.1.2.1 Higher Resolution

Increasing the maximum permissible computational complexity facilitates running LES with greater horizontal and vertical resolution. At present, the highest-resolution LES of atmospheric flows, except for the simulation of cloud chambers, are of the order of 1-m resolution (Matheou and Teixeira 2019).While LES of some cases (particularly those associated with convectively driven turbulence) at substantially coarser resolution have been shown to attain physical fidelity and even to display a degree of statistical grid convergence (Matheou et al. 2011, Sato et al. 2018, Sullivan and Patton 2011), simulations involving suppression of turbulence length scales by stable stratification often require very high resolution to achieve similar fidelity and grid convergence. Such suppression of length scales is commonly found in the atmosphere, for example, in the stably stratified free troposphere surrounding convective clouds, within stable boundary layers, and at the entrainment interfacial zone in stratocumulus-topped boundary layers (Wood 2012). Suppression of turbulence length scales is a challenge for LES, as it is an assumption of the approach that the largest turbulence length scales are resolved by the model. Simulations at this high a resolution are at the limit of what is computable and are far from routine. Due to their immense computational expense, such simulations are often highly idealized, making doubly periodic assumptions and using relatively simple, if any, cloud microphysical process representations.

Over the next five to ten years, it will be important for the LES community to focus on achieving statistically grid-converged solutions for a broad range of conditions, including those with strongly suppressed turbulence length scales. The great computational complexity of such simulations will likely require the continued use of simplified lateral and surface boundary conditions, representations of radiative transfer, and microphysical process models. Even with these simplifications and idealizations, statistically grid-converged LES will provide a useful benchmark or ground truth for the development of subfilter-scale (SFS) closures to be used in coarser-resolution LES as well as in coarse-resolution numerical weather prediction (NWP) and climate models (e.g., Bogenschutz and Krueger 2013, Griffin and Larson 2013, Witte et al. 2022). It will be particularly beneficial to focus efforts on accounting for the effects of stable stratification in SFS models, yielding new opportunities for advancing process science in such conditions. Moreover, statistically grid-converged LES will provide unique opportunities to understand the dynamics of 3D atmospheric turbulence with unprecedented detail. Such data sets would also be highly valuable for machine learning on scale interactions, e.g., energy and momentum transfer across turbulence spectra.

Increasing resolution of LES will also enable better simulation of cases where small-scale surface heterogeneities drive shear instabilities and where thermodynamic gradients are critical. Such cases include 1) simulations involving the urban environment where buildings obstruct the atmospheric flow and the built environment introduces widely varying surface properties; 2) simulations involving the effects of complex terrain; 3) simulations involving atmosphere/ocean-wave coupling 4) simulations involving vegetated canopies 5) simulations involving wildfires formation and spread, and 6) simulations involving renewable energy production such as wind turbines and solar panels. The connections of these three areas with process studies involving aerosols, cloud, and precipitation are manifold.

Urban modeling is likely to be an especially fruitful application of more computationally complex LES, as the built environment strongly forces the atmosphere mechanically and thermodynamically at very small scales while the resulting atmospheric conditions significantly, and disproportionately, impact disadvantaged groups under some conditions. Urban LES would afford the opportunity to connect process models of air quality (atmospheric chemistry and aerosols) and extreme events (temperatures and wind) with public health models to predict impacts on humans at the sub-neighborhood scale. Such LES would require resolution capable of resolving buildings, vegetated canopies, and street canyons.

High-resolution simulations involving complex terrain will also be fruitful in studying terrain-induced convective initiation and enhancement of precipitation. For example, such simulations could enable modeling watershed/basin-level snowpack accumulation, especially in support of field campaigns like the ARM/ASR-supported Surface Atmosphere Integrated Field Laboratory (SAIL).

The ARM Aerosol Observing System (AOS) and an X-band precipitation radar (XSAPR) are pictured on Crested Butte Mountain in Colorado as part of the Surface Atmosphere Integrated Field Laboratory (SAIL) campaign

2.1.2.2 Larger Domains with Realistic Boundary and Initial Conditions (Realistic LES)

In addition to permitting increases in LES resolution, expanding HPC capacity will drive growth in LES domain sizes. It has long been recognized that as atmospheric doubly periodic LES are run for longer durations, the largest scales of spatial variability can grow up to the domain size itself (de Roode et al. 2004), which can potentially adversely affect the model's solution. While on one hand these increasing spatial scales can be accommodated by increasing the spatial extent of the domain, extending the domain to larger sizes begins to make assumptions of spatially homogeneous initial conditions, surface boundary conditions, and large-scale forcing more tenuous. Further, the greater computational expense of running simulations with larger spatial extent limits the resolution used in these simulations.

An alternative to large domain LES with doubly periodic lateral boundary conditions is to replace these idealized boundary conditions with more general boundary conditions that allow inflow and outflow of variability at the domain horizontal edges. These more general boundary conditions require that the atmospheric state be specified on the horizontal boundaries. Idealized methods such as recirculating planes and grid nesting (nesting the LES within itself) can be used for lateral boundary conditions that can be specified using data from another atmosphere model (e.g., atmospheric reanalysis, numerical weather prediction model, or climate model). Using this approach in conjunction with detailed and realistic treatments of the model's surface boundary condition (e.g., through coupling to land surface model [LSM], representations of terrain, and vegetation/urban canopy models) and realistic initial conditions (e.g., through data assimilation) allows simulation of realistic cases that incorporate large-scale (mesoscale and synoptic) variability entering through the domain edges as well as permitting variability developing within the LES domain to exit through the boundary. In the remainder of this report we will refer to such simulations as realistic LES.

Such approaches effectively turn LES into a high-resolution regional mesoscale model providing opportunities to study processes coupling across micro-, meso-, and synoptic scales. Example applications include boundary-layer cloud organization (e.g., cold-air outbreak or stratocumulus), mesoscale deep convective organization, and feedbacks between small scales and large scales (with two-way nesting). Just like deep convection, shallow convection organizes due to the effects of radiation, land surface heterogeneities (Lee et al. 2019; e.g., Tian et al. 2022), or precipitation (e.g., Seifert and Heus 2013). Recent studies distinguished clear pattern differences in this kind of organization (Stevens et al. 2020). Some of these patterns warrant a combination of high-resolution (10 m in the vertical) and large domains (500 km); a configuration that can conceivably be reached over the next 10 years, assuming that LES models have the capability to run efficiently on exascale clusters.

It is also expected that the growth of these realistic LES will be particularly useful in understanding atmosphere-land-surface interactions and terrain-induced flow, as such studies do not lend themselves to doubly periodic domains. Additionally, using high-resolution climate simulations, such as those provided by DOE's E3SM, to provide boundary conditions to LES will permit atmospheric process studies with realistic climate change forcing.

Further, realistic LES make LES-observation comparisons more direct and offer opportunities to improve synergies between observational and LES modeling work to progress atmospheric aerosol, cloud, and precipitation process studies.

2.1.2.3 Computationally Complex Physics

Increasing HPC resources and lowered constraints on maximum computational complexity will be leveraged to increase the use of computationally intensive process representations and the coupling across such process representations in LES. This is particularly true for graphics processing unit (GPU)-based HPC, where simulations become more memory bound than runtime bound, thus leaving room for more complex computations. These include wide use of microphysical and aerosol process representations that do not make the simplified size-distribution assumptions underlying bulk schemes. Such process representations include spectral bin schemes (e.g., Khain et al. 2015) for cloud-precipitation microphysics, sectional methods for aerosols, as well as Lagrangian superdroplet methods (e.g., Dziekan et al. 2019, Richter et al. 2021, Riechelmann et al. 2012, Shima et al. 2009). These schemes may also be coupled with detailed representations of atmospheric chemistry including consistent treatment of LES SFS variability (chemical segregation or incomplete mixing) (Li et al. 2021). Wider use of such approaches will enable detailed process studies of the evolution of droplet size distributions and aerosol-cloud-interactions, with implications for the development of climate model parameterizations and studies of geo-engineering. Further, detailed treatments of aerosol and chemistry coupled to models of public health impacts will facilitate incorporation of societal impacts at LES scales, especially in the context of urban modeling.

Moreover, the representation of atmospheric radiative transfer has largely been relegated to one-dimensional (1D) treatments due to the computational complexity of 3D treatments, despite the general consensus that 3D radiative transfer (RT) may play an important role in microphysical turbulence radiation interactions (Klinger et al. 2019) at cloud boundaries that are critical for determining cloud-dynamics, especially cloud entrainment-detrainment processes (Klinger and Mayer 2014). The distribution of surface radiation in 3D RT is also distinctly different from that in 1D, which plays a crucial role in simulating land-atmosphere interactions and cloud organizations (e.g., Seifert et al. 2015).

2.1.2.4 Laboratory (Cloud Chamber) Simulations

Increasing availability of cloud chamber experimental data (e.g., Chang et al. 2016, Shaw et al. 2020) will present an opportunity to evaluate LES at the chamber scale. Such opportunities will be driven by expansion of the use of computationally complex microphysical and aerosol schemes (like superdroplet, spectral bin, and sectional methods) to simulate clouds in a chamber with well-constrained initial and boundary conditions, offering unique opportunities for the development and intercomparison of various microphysics schemes used in LES (Yang et al. 2022). Such synergistic LES and laboratory approaches can also advance our understanding of cloud microphysical processes, enhance the interpretation of laboratory measurements, and further help to design a large-scale aerosol-cloud-turbulence laboratory facility envisioned as especially important to the scientific community (Shaw et al. 2020).

Along with laboratory-scale simulations, another area of potentially important work will likely be simulations that connect laboratory scales with atmosphere scales. There are two orders of magnitude or more in length scale separation between laboratory scales and typical planetary boundary-layer and/or cloud scales (e.g., the boundary-layer depth or cloud height). Small-domain but very high-resolution LES can be used to connect laboratory-scale observations and typical atmospheric LES (with grid resolutions of a few meters). Similarly, large cloud chambers that are roughly the size of one or potentially a few typical LES grid cells may offer a more direct connection between the laboratory and typical LES. For example, subgrid-scale parameterizations in typical LES (such as surface flux and subgrid-scale fluctuations) can be evaluated by high-resolution laboratory LES or direct measurements within a well controlled environment.

2.1.2.5 Novel Approaches to Analysis

New opportunities will be opened by leveraging novel approaches to extracting data from LES and leveraging modern data science approaches for analyzing LES data. In particular, output of Lagrangian statistics (passively following the fluid flow) and flow coherent structure tracking (like storm or cloud tracking) will enable characterizing the time-evolution of simulated air parcels and flow structures respectively (e.g., Heus and Seifert 2013). The approaches will allow unique opportunities to gain process-level understanding of entrainment/detrainment at cloud margins, the life cycle of individual clouds and populations of clouds, and time evolution of aerosol and cloud droplet/particle populations within air parcels (e.g., Hoffmann et al. 2017). Novel analysis approaches could leverage observational platform/system aware model output tools, like aircraft flight path and tower simulators, that provide localized model output at the native temporal frequency of real observational systems to facilitate model observation synergies. Observational platform/system aware model output integrated with detailed observational system simulators will be an integral component of ModEx/OSSE approaches.

New approaches to analysis will also be driven by the need to compute statistics online in models at runtime due to rapidly growing data volumes associated with increases in model domain sizes, resolution, and complexity of physical process representations. This consideration will provide an impetus for LES researchers to consider exploiting new statistical and analysis approaches that are more easily implemented online in models rather than continuing to rely on postprocessing of output fields.

2.1.2.6 Connections to LES for Renewable Energy Applications

LES is already an important component of renewable energy research. It is an important component of resource assessment studies owing to its high temporal and spatial resolution and physical detail and fidelity. Additionally, there is rapidly growing interest in evaluating interaction between renewable energy installations and the surrounding environment. For instance, better understanding of interactions between wind turbine and wind farm wakes and the atmospheric boundary layer under different stability regimes are needed to optimize farm siting and to design control strategies. Increasing LES grid resolution and the inclusion of detailed treatments of the lower boundary condition in LES will open opportunities to leverage advanced LES designed for cloud/precipitation process studies in renewable energy applications. Potential applications could include use of atmospheric LES to assess wind resources (particularly for offshore development with greater prevalence of cloud-topped boundary layers), to characterize hydrometeors that affect turbine blade longevity, and to examine cloud effects on solar energy production. Further, coupling LES to forcing or boundary conditions derived from climate models could enable such renewable energy process studies under changing climatic conditions.

2.2 What Physical Process Representations in LES Limit Research Progress over the Next 10 Years?

All models of a particular system can be arranged into a model-complexity hierarchy (Held 2005). Note that we distinguish between computational complexity, a measure of computational expense, and model complexity, as a qualification of model detail (that is, what processes are represented in the model either explicitly or parametrically). In answering this unifying question, we address how aspects of LES model complexity limit research progress in the coming decade. We will focus on both limitations in existing process representations and those processes that have so far been neglected.

Large eddy simulation (LES) can resolve the complex atmosphere, land-ocean, and engineered system interactions that are key to optimal renewable energy resource assessment.

2.2.1 Cloud Microphysics, Aerosol, Chemistry

To date, most LES studies involving clouds and precipitation have relied on highly idealized representations of cloud-microphysics, aerosol, and atmospheric chemistry. Indeed, LES with any process representation of aerosol and chemistry (e.g., Slater et al. 2020, Tonttila et al. 2017, Wyant et al. 2022) are the exception, not the rule.

Typically, cloud microphysical processes in LES are represented using bulk schemes that assume a particular form of particle size distribution (PSD) for different cloud and precipitation categories such as rain, snow, or graupel. The parameterization works by solving for different moments of the assumed PSD for different categories. The prognosed moments evolve subject to the LES resolved-scale motions and closure terms representing sources and sinks of the moments. The effects of aerosols are typically introduced at the level of specifying aerosol or cloud-condensation nuclei concentrations. Most often, these bulk microphysics schemes when incorporated into LES are inherited from coarser-resolution atmospheric models with limited or no modification.

2.2.1.1 Limitations of Bulk Microphysics

Many of the microphysical moment source terms are uncertain owing to either limited observational constraints or discrepancies between identification of modeled sources/sinks and actual physical processes. An example of the latter issue is the discrete autoconversion of cloud droplets into rain drops that, although an important part of bulk microphysical schemes, does not reflect the continuous evolution of PSDs seen in nature. Typically, bulk scheme microphysical parameterizations for processes like autoconversion are based on empirically derived curves that are fit to limited data sets that are then applied generally, extrapolating outside of the regimes for which they were designed. The artificial split into different cloud and precipitation categories that is the core of the bulk scheme's design introduces the need for many such hard-to-constrain conversion rates. Such parameterization uncertainties present a significant limitation when using LESs with bulk microphysics schemes as training data for machine learning emulators for LES processes, where one wishes for a close connection between the training data and the underlying true physical processes.

2.2.1.2 Limitations of Spectral Bin and Superdroplet Microphysics

To circumvent many of the assumptions underlying bulk microphysical schemes, two approaches that explicitly represent the evolution of PSD are in active use or development. These two approaches are spectral bin microphysics (SBM; e.g., Khain et al. 2015) and superdroplet (SD; e.g., Shima et al. 2009) methods, both of which eliminate the assumed PSD assumptions inherent in bulk schemes but with significant increases in computational expense. This increased computational complexity has prevented the widespread application of these approaches to LES, particularly LES at very high resolution, even for purely liquid-phase clouds. For example, warm-cloud SD methods require potentially hundreds of individually transported superdroplets per grid cell (Shima et al. 2009). Extension of these schemes to mixed-phase and ice clouds is even more limited due to both increased computational complexity and significant process uncertainties associated with mixed-phase and ice clouds (Shima et al. 2020).

Much of the computational expense of these explicit representations of PSD evolution is associated with the advective transport of the information necessary to sufficiently approximate the PSD. In the case of SBM, this is dictated by the number of bins required to accurately discretize the PSD, and in the case of the SD methods, this is the number of notional particles necessary. Note that in the case of SD methods, the advective transport is represented through the Lagrangian transport of notional superdroplets rather than the solution of a flux-form advection equation.

2.2.1.3 Opportunities for Quadrature-Based Moment Methods

Quadrature-based moment methods (McGraw 1997) offer a potential pathway for balancing accuracy and computational efficiency in LES. Quadrature-based methods represent higher-order moments of distributions using a small set of quadrature points (Fierce et al. 2021), thus limiting the number of advected tracers. In contrast, sectional methods require many fixed bins to accurately represent particles and Monte Carlo Lagrangian particle approaches require simulation of ~100 droplets to represent even univariate distributions. Quadrature-based approaches enable efficient representations of multiple particle types, as has been demonstrated through global-scale aerosol simulations (Bauer et al. 2009) and may offer an efficient framework for unifying simulations of multivariate aerosol size-composition distributions with cloud microphysics (Fierce et al. 2017). To date, quadrature-based moment methods have not been applied for the simulation of cloud microphysics or aerosol processing within clouds; their application in atmospheric science has, so far, been limited to a small number of aerosol schemes.

2.2.1.4 Aerosols and Chemistry

The representation of aerosols and atmospheric chemistry are inextricably linked, as new particle formation and aerosol composition changes depend on complicated atmospheric gas and aqueous chemistry. The chemical composition of aerosols plays a fundamental role in determining their hygroscopicity and thus in determining highly uncertain process rates like the activation of aerosols into cloud condensation nuclei. To date, the incorporation of aerosols and chemistry into high-resolution LES is limited due to considerations of computational complexity. Examples include modal schemes (e.g., Wyant et al. 2022), which are the aerosol analog to bulk cloud microphysical schemes, sectional schemes (e.g., Kurppa et al. 2019, Tonttila et al. 2017), which are the aerosol analog to spectral bin cloud microphysical schemes, and SD methods (e.g., Jaruga and Pawlowska 2018). Like the limitations of cloud microphysics, the application of sectional aerosol methods to high-resolution LES has been limited by their computational expense, much of is due to the cost of transporting scalars associated with each aerosol bin. This expense is further compounded when aerosols are coupled to detailed treatments of chemistry involving multiple chemical species, each of which must be transported by the model. Furthermore, both aerosol and chemistry schemes involve coupled source terms operating with a range of time scales that implies the necessity of relying on stiff ordinary differential equation solvers for their time integration; such solvers are notoriously complicated and computationally expensive.

A greatly valuable use case for detailed representation of aerosol and chemistry in LES are the studies of air quality impacts on human health. Air quality depends on accurate predictions of aerosol and trace gasses. High-resolution LES of the urban environment, combining process representations of aerosol and chemistry with models of air quality impacts on human health, would allow unprecedented studies and predictions of how atmospheric processes impact humans and would allow characterization of differential impacts across socioeconomic disparities in urban areas at the neighborhood scale.

A further extension and application of detailed aerosol and chemistry in LES is the injection of aerosol into the atmosphere from wildfires and the subsequent processing of these aerosols in buoyancy-driven wildfire plumes. Incorporation of fire-spread models into LES would facilitate detailed modeling of terrain-fire-atmosphere interactions and their impacts on aerosol injection into the atmosphere as a part of wildfire plumes.

2.2.1.5 Lack of Unified Representations of Aerosol, Cloud Microphysics, and SFS Turbulence

At the physical level, turbulence, cloud microphysical, aerosol, and atmospheric chemistry processes are inextricably linked. Take, for example, the production of aerosol via the evaporation of cloud droplets. The size and composition of these cloud-processed aerosols depend on the growth history of evaporating droplets. This combines the effects of aerosol activation with the effects of chemical reactions inside cloud droplets. Aerosol activation depends on the existence of supersaturation, which is largely determined by atmospheric turbulence and the chemical composition of the original condensation nuclei. The chemical reactions inside cloud droplets depend on the concentrations of dissolved chemical species in the aqueous phase which, in turn, depend on the aqueous-phase chemical reactions between them and the evolution and eventual evaporation of cloud droplets. Precipitation adds another layer of complexity to this cycle, by introducing highly non-linear effects of collisions between aerosol containing water drops. All of these processes physically occur at scales that are inherently sub-filter scale even to LES and thus must be parameterized.

At present the microphysical, aerosol, chemistry, and SFS turbulence schemes widely used in atmospheric LES are coupled, at best, at the grid scale. That is, most often the process representation used in LES typically depends on resolved (grid cell mean) quantities, thus ignoring SFS variability. It is widely appreciated that for process representations that are non-linear, ignoring such variability introduces model biases (e.g., Abade et al. 2018).

2.2.2 Surface Boundary Conditions

A key component of atmospheric LES is how the model's lower boundary condition is specified; numerically most models use free-slip boundary conditions on the horizontal velocity components and no penetration conditions on the vertical velocity. With these numerical boundary conditions, there is no scalar or momentum flux through the lower boundary. However, it is through this boundary that the atmosphere interacts with other components of the Earth system, for example, the effects of surface roughness and topography, vegetation, water bodies, or even the built urban environment.

Idealized LES, like those that form the basis of most intercomparison studies, have largely relied on simplistic representations of the lower boundary. These have included specifying surface fluxes of momentum and scalar quantities directly, specifying drag coefficients and surface temperature and using bulk aerodynamic formulae to compute fluxes, or specifying surface roughness and temperature and using Monin-Obukhov similarity theory to compute drag coefficients for use with bulk aerodynamic formula. Typically, these approximations assume significant horizontal homogeneity at the surface well beyond that typically seen in nature.

2.2.2.1 Limits of Monin-Obukhov Similarity

Concerns exist regarding the parameterization of surface fluxes in LES using Monin-Obukhov similarity. First, Monin-Obukhov similarity is formulated in the context of long-timescale or large-spatial-scale ensemble-like statistics, while often in LES it is applied to represent SFS-fluxes that are far from this statistical regime. To make this point clearer, application of the Monin-Obukhov similarity would be more appropriately applied to LES domain mean fluxes rather than grid scale fluxes as is typically done. Moreover, Monin-Obukhov theory involves the specification of parameters that have been determined empirically and for a relatively narrow range of conditions but are applied broadly in LES.

2.2.2.2 Surface Models

LES have also been coupled to surface energy balance models, taking the form of either highly idealized energy balance models (e.g., Lee and Khairoutdinov 2015, Tan et al. 2016) or more complicated land surface models often inherited from coarser-resolution models (e.g., Fast et al. 2019b, Pressel and Sakaguchi 2021). While these approaches provide spatially heterogeneous and/or energetically consistent treatments of surface fluxes, they typically rely at some level on Monin-Obukhov similarity-like assumptions and thus suffer from similar limitations. That said, the use of these approaches has underscored the importance of accurate and energetically consistent surface flux representations.

2.2.2.3 Topography

Many atmospheric LES involving variations in topography have been performed using models with terrain-following coordinates. Most often, these LES are conducted using models originally designed as mesoscale numerical weather prediction models but run at LES resolution. At the high spatial resolution of LES, terrain-following models are known to be adversely affected (in terms of accuracy and numerical stability) by large gradients of terrain, so much so that many models rely on artificial spatial smoothing of the terrain to maintain stability. Such smoothing may present a significant limitation to resolving flows in highly complex terrain – for example, studies of convective initiation over mountainous terrain.

2.2.2.4 Embedded Terrain and Vegetation Canopies

An alternative to terrain-following coordinates is the use of immersed or embedded boundary methods (Iaccarino 2005). Note that such approaches can be used in replacement of or in conjunction with terrain following coordinates. These methods have proven to be particularly well suited to representing large gradients in surface height even to the point of resolving flows in complex urban geometries. There are a range of approaches to implementing immersed boundaries ranging from simple filled-cell methods (e.g., Khairoutdinov et al. 2022, Muñoz-Esparza et al. 2020, Maronga et al. 2015) that treat LES grid cells as all atmosphere or all terrain to methods that represent the flow effects of terrain that only fractionally occupies grid cells (e.g., Auguste et al. 2019, Lundquist et al. 2010, 2012). While these approaches offer significant flexibility in the representation of complex terrain and structures in atmospheric LES, their implementation is non-trivial and at present is only available in a limited number of models. Moreover, as they are a non-trivial modification to the model, leveraging existing land surface models at the same time as embedded boundary methods is not straightforward. This is especially true in the context of urban LES in which buildings are resolved using immersed boundary methods, thus potentially requiring thermodynamic fluxes to and from buildings to be represented through coupling with a building energy model (e.g., Maronga et al. 2015). Such coupled atmosphere-building modeling approaches that are required uniquely by LES are still in their infancy, and their development is impeded by the limited availability of high-quality observational data needed to evaluate them. Note that such process models are uniquely required by LES, because they are only relevant to models capable of running with sufficient resolution to resolve the flow around built structures.

A related issue to embedding of terrain and/or the built environment within LES domains is the representation of the atmospheric flow and its two-way coupling with vegetation canopies. At present LES vertical resolutions of < 10 m near the surface, forest canopies can be resolved within LES, given a parameterized representation of the effects of the forest on the atmospheric flow. The effects include the representation of forests decelerating the atmospheric flow, providing elevated sources of sensible and latent heat flux associated with absorption of radiation and plant evapotranspiration, and radiative extinction within the canopy layer. Note that the approaches stand in contrast to 1D multi-layer canopy models that represent such effects in land surface models in that they resolve the interactions of plant canopies with the fully 3D LES-resolved atmospheric flow (e.g., Kanani-Sühring and Raasch 2015, Yue et al. 2007, Ma and Liu 2019). Like atmosphere-building energy modeling approaches, such atmosphere-plant canopy representations are uniquely required by LES due to their high resolution.

2.2.2.5 Wildfire Modeling

Another, more extreme, surface boundary treatment for LES that would open new opportunities for advancing process science as well as for studying human impacts is wildfire-spread models. Wildfire spread models represent the surface fluxes of heat, water, and smoke into the atmosphere associated with the combustion of

Integrated large eddy simulation (LES) wildfire modeling presents opportunities for a process-level understanding of wildfire dynamics and their influences on aerosol-cloud interactions.

biomass, and the effects of the atmosphere on driving wildfire spread. Such models are already integrated into mesoscale models (e.g., Weather Research and Forecasting [WRF]; Mandel et al. 2011, 2014) but integration of the models into LES with detailed representations of terrain would allow resolving details of wildfire, terrain, and atmosphere interactions with unprecedented detail. In the context of aerosol-cloud-precipitation process studies, wildfires are a significant source of atmospheric aerosol and the injection of those aerosols into the atmosphere depends on the dynamics of the buoyancy-driven wildfire plumes that in turn depend on surface fluxes of buoyancy arising from biomass combustion.

2.2.3 Radiative Transfer

To date, LES have largely relied on 1D representations of radiative transfer. While at the coarse grid resolutions used in numerical weather prediction and climate models a 1D approximation is likely appropriate, the same may not be true in high-resolution models like LES that resolve cloud morphology because 3D radiative effects at the edges of clouds may influence cloud processes like entrainment/detrainment. Further, 1D approximations are also limiting because the effects of solar angles on the shadow cast by clouds are not accounted for, which can alter surface energy balances. Additionally, in deep convection 3D radiative transfer is known to significantly alter radiative heating rates in both the cloud and surrounding clear regions (Di Giuseppe and Tompkins 2003). In the context of urban modeling, 3D radiative effects likely play an important role in determining neighborhood-scale temperature extremes as well energy balances within the built environment.

3D radiative transfer has been avoided because of its significant computational expense. A good deal of that expense is associated with the parallelization of atmospheric models. Most, if not all, atmospheric models are parallelized in horizontal directions such that vertical columns reside locally in memory: thus radiative transfer is trivially parallel and requires no additional communication. The same is not true for 3D radiative transfer, which is not trivially parallelized and requires additional parallel communication. Approximate representations of 3D radiative transfer have been developed (e.g., Jakub and Mayer 2015, 2016), but they are in general significantly more expensive than 1D treatments. Recently, machine learning techniques have been used to expedite 3D radiative transfer, either parameterizing 3D radiative effects (Meyer et al. 2022) that are then added to 1D radiative transfer output, or directly confronting 3D radiative transfer specifically designed for low-topped clouds at LES resolutions (Veerman et al. 2020).

2.2.4 SFS Models

LES rely on SFS models to represent the effects of unresolved turbulent processes on the resolved scale flow. The most widely used approaches to SFS modeling include Smagorinsky-type and turbulence kinetic-energy type closures. However, the development of novel SFS closures is an active area of research. A major limitation of many SFS models is their representation of the effects of stable stratification, for example, in the case of stable boundary layers or at stable inversions at the top of the planetary boundary layer. Physically, in conditions of stable stratification, turbulence length scales are strongly suppressed, so much so that the largest scales may be smaller than the model's filter scale. When this happens, LES is no longer able to resolve the largest energy-containing scales of motion, which is a fundamental assumption of LES. Moreover, many LES SFS models explicitly suppress the effects of SFS turbulence in the presence of strong stratification, often for rather ad hoc reasons. Taken together, this has the effect of making it very difficult to achieve high-fidelity LES of stable boundary layers. Currently, higher-order closure schemes are relatively uncommon in atmospheric LES because increasing the resolution often yields better results for the same increase in computational cost. With

LES becoming more memory bound on GPU-based HPC, it may be worthwhile to revisit higher-order closure schemes.

Another practical challenge of SFS modeling in LES is that it is difficult to disentangle numerical error associated with the implementation of the model's advection schemes from the effects of the model's SFS closures for both scalars and momentum. Understanding these interactions has proven to be decisive for high-fidelity simulations of some boundary-layer and cloud types, like stratocumulus (e.g., Pressel et al. 2017). These interactions between SFS models and model numerics may limit the generality of SFS models when applied across diverse cloud types and may prove critical in determining the ability of LES to represent key atmospheric processes. As the role of SFS modeling becomes less important with increasing LES resolution, grid convergence studies are an ideal experimental platform for understanding the effects of numerics and SFS models on LES. To date, due to their significant computational expense, there have been no large-scale multi-model LES convergence studies.

2.2.5 Balancing Computational Complexity between Physical Detail and Resolution/Domain Size

A factor in nearly all these process representation limitations is computational complexity. Given finite computational resources, the weighing of computation complexity associated with process representations against computational complexity associated with domain size and grid resolution will be a determining factor in using LES for process science over the next decade and beyond. Moreover, changes in computational hardware and software design strategies will play a role in determining this balance.

2.3 What Aspects of Current LES Implementations Will Limit Research Progress over the Next 10 Years?

2.3.1 Hardware Advances and Portability

Over the next decade, it is expected that high-performance computing code like LES will run on 2-4 exaflop machines. These new exascale computer systems, such as Frontier, rely on GPU-based or APU (Accelerated Processor Unit) hardware. This creates new challenges and opportunities because most existing codes do not provide hardware portability between CPUs and GPUs.

On the opportunity side, we will be able to fully resolve many boundary-layer and turbulence processes (<5m), expand to much larger domains to better understand interactions and organization at the mesoscale (>100 km), or add complexity beyond the traditional focus on turbulence, for instance, by including chemistry, more sophisticated microphysics, or 3D radiative effects.

Since idealized LES codes, with simple physical process representations, are typically much less complex than large-scale models, porting existing codes to new architectures or writing entirely new hardware portable LES codes may be significantly easier than for large-scale models. That said, making efficient use of GPUs requires hardware portability of all physical process representations, which significantly increases the effort required for the development of hardware-portable LES codes that include detailed process representations. Several proprietary (e.g., CUDA) and open (e.g., openACC, HIP) frameworks, as well as some generalization layers (e.g., Kokkos), and high-level languages like Python or Julia that offer several approaches to achieving hardware portability, are available to facilitate portability between different types of hardware, and it makes sense to promote the use of these layers. However, it is not yet clear how that environment will equilibrate, and what best practices will look like over the next decade.

Many LES codes are maintained by small teams without a clear funding structure to support them, which obviously makes it harder to rewrite LES codes. Perhaps the greatest obstacle for developing hardware portable LES codes, either from existing LES codes or entirely new codes, is a lack of the software engineering expertise to complete the tasks. DOE/BER has an opportunity to help develop these best practices through the generation of a broad knowledge base.

Another challenge of GPU-based computing is that, at least currently, GPUs tend to be more memory bound than compute-time bound. Moreover, GPUs suffer from significant host-to-device memory copy overhead that can significantly cut into GPU performance gains, especially with multiple GPU deployments that rely on communications over message passing interface (MPI). Such multi-GPU implementations are necessary to effectively use DOE's new HPC resources and to accommodate LES process representations with large memory footprints (e.g., spectral bin microphysics, sectional aerosol methods, and chemistry). While this may change in the future, it suggests that the current computing environment is particularly well suited for the following type of experiments:

- High-resolution experiments, as opposed to large domain, since a resolution doubling requires 16x the compute power/8x in memory versus a horizontal domain doubling that scales 4x in compute and 4x in memory usage
- Long-duration experiments
- High-complexity experiments, such as sophisticated radiation or advanced SFS models and process models that do not significantly impact the model's memory footprint.

A large component of the significant effort required to develop hardware-portable LES codes is developing hardware-portable physical process representations (e.g., land surface model or aerosol-cloud interactions) that historically have been leveraged from coarse-resolution models. Thus one perspective on the need to develop hardware-portable physical representations is that it is an opportunity to start from scratch and build hardware-portable, LES-specific, process representations, rather than porting existing code bases from coarse-resolution models.

2.3.2 Programming Languages and the Democratization of Atmospheric Models

Historically, atmospheric models have been implemented in Fortran, which for decades has been the de facto language of high-performance scientific computing. Over the last decade, however, the trend has been to do new atmospheric model developments in languages other than Fortran, for example, C++ (e.g., Bertagna et al. 2019, Caldwell et al. 2021, van Heerwaarden et al. 2017), Julia (e.g., Sridhar et al. 2021), or Python (Pressel et al. 2015, Pressel and Sakaguchi 2021).

While there are many reasons for this trend, three seem particularly important. First, other languages, or extensions to them, are becoming comparably performant to Fortran. Second, the greater levels of abstraction afforded by these languages make it easier to achieve hardware portability either through direct access to GPU programming languages like CUDA or through packages like Kokkos (Trott et al. 2022), CuPy (Okuta et al. 2017), or Numba (Lam et al. 2015). Further, additional abstraction in theory can make codes more extensible. Third, some languages, for example, Julia or Python, make models accessible to a broader community of users and open the community to the new generation of developers with modern computer science training. The expansion of the community of users and developers is in direct analogy with the democratization of machine learning (Chollet 2017) that has been used to describe the rapid progress of that field afforded by the development of highly accessible tools in unified languages. The example set by the machine learning community could be extended in the atmospheric science community to the notion of the "democratization of atmospheric models".

The pros of a democratization of atmospheric models are particularly evident in the case, as in machine learning, of Python. First, Python is one of the most widely taught languages at the collegiate level and is among the most widely used languages for routine analysis by atmospheric scientists, making the pool of Python-fluent people who can contribute to model development larger than for other languages. A limited pool of developers can be a complicating factor for the development of models in other languages, such as C++ or Julia. Second, models written in Python allow scientists to unify their modeling and data analysis workflows seamlessly within the context of a single programming language, potentially increasing their productivity and confidence in extending the model.

Democratization of atmospheric models in Python also provides opportunities for students to build highly marketable software engineering skills in a widely applicable programming language.

2.3.3 Data Management and Data Transfer

With common data sets soon reaching terabyte sizes and more, transfer of data over the internet quickly becomes a limiting factor. Common data archives and onsite post-processing toolkits based on cloud-native libraries (e.g., Pangeo [https://pangeo.io/] or XArray [Hoyer and Hamman 2017]) could significantly mitigate these issues and make the data more freely available across the scientific community.

LES, like most atmospheric models, are input/output (IO) intensive: that is, models typically output large volumes of data at high frequency, which contributes to making output a non-negligible component of model runtime. IO performance is very sensitive to many factors including aspects of algorithm and software design as well as HPC hardware and system/network load, thus making IO performance tuning difficult. IO performance is also highly dependent on aspects of the simulation like domain size and resolution and the number of output fields. These challenges mean that most LES are run with relatively little IO performance tuning, in part because such tuning is time consuming and needs to be done on a system-by-system and problem-by-problem basis. Automated IO performance tuning strategies could reduce the burden of IO performance tuning placed on LES users and allow them to more effectively use HPC resources. Such automated approaches may prove particularly useful as the importance of optimizing IO will likely increase in the future as increasing model performance and domain sizes resulting from advances in hardware may lead to IO taking a relatively larger portion of the model runtime.

A significant portion of the time spent by models doing IO is associated with outputting the model's 3D fields, and thus an obvious strategy for reducing IO time is reducing the total number of 3D fields output by the model. One approach is to compute as many derived (reduced dimension) statistics and diagnostics as possible online within the model. A particularly worthwhile effort would be to identify a standardized and exhaustive list of such reduced dimensional quantities to be output in models, in conjunction with naming and storage conventions. Even if the model output is not fully in compliance with a standard, the mere existence of such a standard would encourage and facilitate the development of conversion scripts into this common standard.

2.3.4 Model Equations

An important consideration in the design and formulation of LES codes is the model's governing equations. Choices made regarding these equations directly impact both the model's throughput (how long it takes for a model to integrate forward in time a given amount) and the model's generality. Historically, atmospheric models designed from the outset to be LES codes have typically adopted governing equations that, through various approximations, eliminate acoustic modes from the model's solution. The reason is that at LES resolutions of tens of meters, the phase speed of the acoustic modes (i.e., the speed of sound) strongly limits the maximum stable timestep (set by the Courant Friedrichs Lewy [CFL] stability criterion) permitted for explicit time integration of the equations of motion. As the acoustic modes are typically assumed to be dynamically unimportant, many LES codes seek to remove them from the solution so that the maximum stable time step for a given resolution is set by, essentially, the fluid velocity. Eliminating these acoustic modes is achieved typically by making the incompressible, Boussinesq, anelastic, or pseudo-incompressible approximations. These approximations are colloquially referred to as "sound-proofed" approximations. Of these approximations, the anelastic approximation has been the most widely used by atmospheric LES bcause it allows accurate simulation of even deep convective motions (Kurowski et al. 2014) while permitting a computationally efficient solution to its mass continuity equation, for example, using direct Fast Fourier Transform-based fast solvers.

Non-hydrostatic mesoscale models, like WRF, typically solve the compressible equations of motion, and usually employ time-splitting algorithms and implicit time integration of the vertical component of the momentum equation to make simulations computationally tractable. The reason for the separate treatment of the vertical component of the momentum equation is that mesoscale atmospheric models typically employ much higher vertical grid resolution (typically 10s of meters) than horizontal grid resolution (typically kilometers), so that the vertical resolution would strongly limit the maximum stable time step, due to the CFL stability constraints, if it were explicitly integrated in time. However, when models like WRF are run in LES configurations where the horizontal grid resolution is comparable to the vertical grid resolution, the maximum stable time step is again highly limited by explicit integration of horizontal acoustic modes and the CFL criterion.

At LES resolution, all other things being equal, the differences in model throughput for a "sound proofed" model versus a compressible model can differ by an order of magnitude or more. Atmospheric models based on anelastic and pseudo-incompressible governing equations can be designed with general lateral boundary conditions (not just doubly periodic), terrain-following coordinates, and grid nesting in a similar fashion to fully compressible models (e.g., Lac et al. 2018). However, as with any approximation, there are compromises. In the case of the anelastic equation set, terms in the vorticity equation are truncated that may become important at near-planetary scales (Kurowski et al. 2015). These truncated terms have been shown to be important in idealized moist baroclinic instability problems where, based on dimensional analysis, one would expect the truncated terms to be significant. However, it is not clear that for more realistic problems these missing terms would be detrimental. Note that the anelastic system is already being used with success globally.

Given the scientific opportunities presented by both high-resolution LES, for which "sound-proofed" models are likely to be computationally more optimal, and for large-domain realistic LES for which the limits of some "sound-proofed" models may be reached, it will be beneficial to conduct detailed observational evaluation of "sound-proofed" models for real cases. This is especially true in multiscale simulations.

2.3.5 Benchmark Cases

A critical aspect of model development and evaluation is the simulation of benchmark cases. These cases allow checking that model developments yield realistic results and/or results that are easily comparable with other models. Moreover, comparing simulation of benchmark cases between models increases confidence in the use of LES in process studies. Historically, such benchmarks have been in one of two forms, either idealized 2D cases, like density currents (Straka et al. 1993), positively buoyant bubbles (Bryan and Fritsch 2002), or squall-lines (e.g., Bryan and Morrison 2012), or idealized cases that have formed the basis of canonical LES intercomparisons studies that are to varying degrees based on observed cases with highly idealized forcing (Ackerman et al. 2009). Here we identify several strategies that could increase the impact of benchmark cases on model development and more generally in growing confidence in the application of LES to process science.

2.3.5.1 Statistical Grid Convergence

Increasing HPC resources will make grid-converged LES more readily attainable over the next decade. To date, only a few 3D LES studies have been able to achieve statistical grid convergence (e.g., Matheou and Teixeira 2019, Sato et al. 2018, Sullivan and Patton 2011). Development of a diverse set of LES cases that reach statistical grid convergence will give the opportunity to evaluate models independent of grid-resolution sensitivity, thus enabling comparison of models' sensitivity to microphysical processes and providing benchmarks for development of SFS closures for LES performed at coarser resolutions.

2.3.5.2 Revisiting Canonical LES Intercomparison Cases

Another potentially fruitful allocation of effort, given advances in LES techniques and growth in HPC resources, is to revisit existing canonical LES intercomparison cases (Ackerman et al. 2009, Siebesma et al. 2003, Stevens et al. 2005, vanZanten et al. 2011). Many of the widely simulated LES cases are based on intercomparisons that are now more than a decade old. Establishing new intercomparisons among models based on these cases would afford opportunities to document progress in the field and identify current deficiencies in models given modern LES and HPC resources. Revisiting such cases in the context of statistical grid convergence as mentioned above may be particularly useful. Further, many of the canonical LES intercomparison cases do not include adequate specification of the aerosol and/or microphysical state required to initialize and run modern microphysical process models, so extending the original case specification to include this information would allow opportunities for intercomparison of LES with a wider range of process models.

2.3.6 Long-Term Support for Source Code Management, Software Availability, and Releases

The scientific community broadly supports adoption of open-source software paradigms based on distributed version control platforms like GitHub, Bitbucket, and Gitlab. This paradigm enables adoption of software development best practices including code review, software testing, issue tracking, and rigorous documentation. Further, open-source development enables transparency in model implementation, reproducibility, and the democratization of modeling through increased code availability. For these reasons scientific journals are increasingly moving towards or are requiring articles to make modeling software openly available with explicit release version numbers and digital object identifiers (DOIs) prior to publication.

However, open-source software necessitates increased and long-term support to manage merge requests, software testing, software builds, curate documentation, provide user support, and manage formal software releases. As LES software infrastructures grow, it becomes increasingly difficult for small teams with short-term support to manage these tasks.

2.3.7 Community versus Small-Group Models

Another topic that emerged during the workshop regarded the division of effort between models developed, supported, and used by large communities of users in the same vein as the WRF model, and models developed and used by small teams.

The advantages of community models include:

- The opportunity to leverage the talents of a larger group of developers and users, to rapidly build model capabilities especially for representation of diverse processes.
- Avoidance of duplication of effort.
- Providing a platform for collaboration across disciplines.
- Focusing efforts of software engineers to support hardware portability, especially on DOE exascale systems.

The advantages of small-group models include:

- Increased model diversity.
- Smaller, perhaps more understandable, code bases result in more conceptual insight.
- Increasing the number of people in the community with experience in low-level, fundamental model development.

A further perspective provided by some at the workshop is that the small-group models will likely continue to support mostly idealized, although still important, modeling studies, due to the additional development burden necessary to provide process representations and model generality necessary to support realistic LES. While some small-group models will undoubtedly make the transition to realistic LES, progress will likely be slower than community efforts.

While a future of both community and small-group development seems likely, at present there is no clearly identifiable community model within the United States tailored to atmospheric LES in support of atmospheric aerosol, cloud, and precipitation process studies. WRF is perhaps the model most closely fitting this bill, as it is routinely used for LES; however, due to its compressible dynamical core, model throughput is severely degraded at LES resolution relative to models that solve 'sound-proofed' equations.

Development of a community model for performing both idealized and realistic LES needs long-term support to address the software development best practices discussed in Section 2.3. Moreover, it would be beneficial to complete such development within a fully integrated community of software engineers, process scientists, observational scientists, and large-scale (climate) modelers leveraging the expertise of each group and to ensure that the model meets the needs of stakeholders.

Assuming, as seems likely, that both community and small-group models persist into the future, it seems important that both adopt software best practices that streamline sharing of source code, particularly of physical process representations, between models. This would potentially accelerate the development of idealized small-group models into realistic LES.

2.3.8 LES Integrated with Data Assimilation

A topic of significant discussion during the workshop was the integration of data assimilation techniques into LES. Incorporation of data assimilation may be important for realistic LES applications. Significant questions were raised about the appropriateness of data assimilation at LES scales, what fields and observations should be assimilated, and at what scales the assimilation should be applied. At present, few LES codes and studies have incorporated data assimilation, especially at LES scales, and doing so would likely require substantial fundamental research and software development.

2.4 What Kind of Observations Would Be Useful in Improving and Further Validating LES?

Observations are needed to facilitate improvement and validation of LES. The data collected during multi-platform, large field campaigns have been used to create canonical cases through intercomparison studies, such as Dynamics and Chemistry of Marine Stratocumulus (DYCOMS), Barbados Oceanographic and Meteorological Experiment (BOMEX), Atlantic Trade-Wind Experiment (ATEX), and Atlantic Stratocumulus Transition Experiment (ASTEX) (van der Dussen et al. 2013, Siebesma et al. 2003, Stevens et al. 2001, 2005). ARM observatories or field campaigns provide long term, high-resolution measurements of aerosol, cloud, dynamic, radiative, and thermodynamic fields and have been used for improving and validating LES models aimed at studying cumulus clouds and land-atmosphere interactions, mixed-phase clouds, and marine stratocumulus clouds, e.g., Routine AAF Clouds with Low Optical Water Depths (CLOWD) Optical Radiative Observations (RACORO; Endo et al. 2015), Indirect and Semi-Direct Aerosol Campaign (ISDAC; Ovchinnikov et al. 2014), Marine ARM GPCI Investigation of Clouds (MAGIC; McGibbon and Bretherton 2017), Holistic Interactions of Shallow Clouds, Aerosols, and Land-Ecosystems (HI-SCALE; Fast et al. 2019a), and the Land-Atmosphere Feedback Experiment (LAFE; Wulfmeyer and Turner 2018).

Over the past few decades, atmospheric measurements have experienced incremental improvements in observational technology. Specifically, the samplings of observation systems are often not dynamically oriented. In other words, the measurements are not optimally sampled when and where needed. This is largely due to 1) scale mismatch in that the current resolutions of instruments cannot reach to the native scales of the key small-scale processes controlling climate sensitivities such as aerosols, clouds, and precipitation; and 2) lack of spatial representation in that measurements are not all inclusive to provide information representing vertical motions (e.g., in clouds), heterogeneities (e.g., land surface and across different processes and regimes), and temporal evolution (e.g., transitions across regimes or life cycles of systems).

Listed below are some of the needs together with the current state of the observations and possible ways to improve them.

2.4.1 Continuous Measurement of High-Resolution Vertical Profiles

First, we need continuous measurements of high-resolution vertical profiles of 1) thermodynamic state variables such as temperature, water vapor mixing ratio, and wind fields, especially those in the boundary layer and the lower troposphere where there is a sharp gradient that limits the boundary-layer growth or mixed-layer growth, e.g., across the layer at the top of the stratocumulus cloud layer or boundary-layer top or in between sparse cloud fields; 2) PBL top and turbulence moments such as vertical velocity, heat or water vapor or hydrometeor variances, and vertical fluxes both in sub-cloud layers and cloud layers; 3) aerosol composition and size distributions, cloud condensation nuclei (CCN), ice nuclei (IN), and cloud droplet number concentration; 4) in situ or remote-sensing data of cloud properties for in-cloud buoyancy sorting and variabilities such as Paluch mixing line such as from flight data.

Sounding data two or four times a day is far from enough. For convection triggering or cloud onset, we really need measurements within one or two hours ahead of the event occurrence to determine the environmental conditions and controlling mechanisms. Many of these data needs call upon the co-located measurements of high-resolution

Radars and lidars, foreground, are located near the Guest Instrument Facility, left, and the optical trailer at ARM's Southern Great Plains Central Facility near Lamont, Oklahoma.

vertical pointing instruments including Aerosol Observing System (AOS) systems (Beamesderfer et al. 2022, Helbig et al. 2021), Doppler lidar, Raman lidar, cloud radar, wind profiler, and so on, and retrieval algorithms for combining measurements across different instruments, e.g., for water vapor turbulent fluxes. ARM observatories, such as Southern Great Plains (SGP), are good examples of this, especially due to the advanced development in the past decade. The Global Energy and Water Exchanges (GEWEX) Global Land/Atmosphere System Study (GLASS) panel's new project, the GEWEX Land-Atmosphere Feedback Observatory (GLAFO; Wulfmeyer et al. 2018, 2020) is advocating along this line for the systematic enhancement of profiling capabilities from bedrock to the top of the planetary boundary layer.

2.4.2 Spatially Distributed Measurements of Heterogeneities

Second, we need spatially distributed simultaneous measurements to fully understand the coupling processes between land/ocean surface, boundary layer, aerosol, and clouds/precipitation. This not only requires measurements over different land surface conditions including soil properties, land cover/use, vegetation types, topography, coastlines, and urban effect, but also requires consideration of the patterns and the length scales of the land surface heterogeneity, which may induce secondary circulations and cause static or dynamic impacts on aerosol processes and clouds/precipitation (Lee et al. 2019, Tian et al. 2022). Such data will require co-located atmospheric and land/ocean surface measurements accounting for the effects of land surface heterogeneity and its induced secondary circulations. In land atmosphere interaction studies, it often requires a distinction between local and non-local effects, as for the dominance of controlling mechanisms. In this sense, a carefully designed network of sensors with boundary-layer profiling capabilities is needed, not only to represent mesoscale spatial variability, but also to characterize the regional advections and water recycling.

2.4.3 Statistics of Ensembles of Canonical Cases

Third, we need observational statistics from well-designed classifications of observations. For example, ensembles of "golden days" cases, instead of a few canonical cases, are needed to sample a comprehensive spectrum of climate, clouds/precipitation regimes, especially those regimes associated with extreme conditions or events. Parameterized schemes often need calibrations for their empirical coefficients; however, compensating errors are often roadblocks of parametric calibrations for optimal performance. We should carefully construct these ensembles not only to represent different regimes, but also to be hierarchical, i.e., to tackle the processes and the corresponding parameterized representations step-by-step from simple (such as clear-sky turbulence cases) to complex (such as mesoscale convective aggregation cases). Such ensembles of cases should become a shareable case library for LES validation. Another example, an extraction of observed variable relationships, is needed instead of comparisons of variables alone, such as covariance both temporal and spatial, or cause-effect or lead-lag and so on. If such relationships exist, we should include them into a standard diagnostic package for LES as the first checkpoint on its performance.

2.4.4 Morphology of Individual Cloud and Precipitation Clusters

Fourth, we need four-dimensional (three spatial dimensions plus time) morphology measurements of individual cloud and precipitation clusters for LES validations. This requires measurements of high frequency (minutes) and large areal coverage, e.g, at least, several or a few tens of kilometers for shallow cumulus and a few hundreds of kilometers for mesoscale organization of shallow and deep convection. In addition, tracking algorithms are needed to trace these individual clusters' life cycle evolution. In such comparisons of statistics, instrument simulators are often needed to facilitate apple-to-apple validations.

2.4.5 Cloud Chamber Experiments

Fifth, we need cloud chamber measurements to evaluate and constrain microphysical processes in LES. Convection cloud chambers, which can generate and maintain steady-state clouds for several hours, allowing the measurements of cloud properties in detail, have shown huge potential to explore aerosol cloud-turbulence interactions. High-resolution LES is a perfect tool to simulate steady-state turbulent clouds in a convection chamber. Relatively simple chamber model setup with observationally guided and well-constrained initial and boundary conditions can help to identify and attribute the source of uncertainties in the algorithms of microphysical schemes. Laboratory measurements of the means and fluctuations of dynamic, thermodynamic, and microphysical properties in a large cloud chamber can also help to constrain and evaluate SFS modeling in LES.

Finally, uncertainties need to be quantified for the observational data used in LES validation. This is important for us to understand both observation qualities and model performance. Such uncertainties include instrument sampling errors, systematic bias corrections, multiple instrument measurement differences or definition differences (e.g., planetary boundary-layer [PBL] top), case spread in ensembles, simulator assumption inconsistencies, tracking algorithm random errors and uncertainties, and so on.

2.5 How Do You See Possible Improved Synergy between Observations and LES in Studies of the Atmosphere, and What Are the Challenges in Doing So?

Due to the high level of effort and skill needed to gain expertise in either LES models or observations, the scientific communities using these tools to study atmospheric phenomena were, to some extent, decoupled. Here, by observational scientists we mean scientists who use data collected by instruments to study atmospheric processes, and those who develop new retrieval techniques to derive atmospheric (cloud, aerosol, thermodynamic) properties using collected data. In the past decade or so, however, LES modelers and observationalists on process studies have been working hard to bridge the gap. The collaborations between the two communities may flow naturally in a few pathways.

2.5.1 Golden Day Library of Large-Eddy Simulations and Observations

While idealized LES, for example with domain mean forcing and doubly periodic lateral boundary conditions, are still very attractive and important for process understanding, we may need to pay more attention to the connections between LES and observations, in that often our LES's setup, configuration, boundary conditions, and large-scale forcings may be far from the reality in observations (Schemann et al. 2020). Idealized LES tests will guide us on missing processes or mechanisms, more realistic LES simulations will complement idealized tests to address the effects of processes or mechanisms to a quantified extent, and such information will be particularly helpful to inform observational strategies, especially taking advantage of the development of instrument simulators and forward model OSSE tools.

Golden day simulations for data collected during field campaigns have become a nexus connecting LES modelers and observational scientists. As compared with the first few model intercomparison cases in the past, e.g., the classical GEWEX Cloud System Study (GCSS) LES/cloud-resolving model (CRM) modeling cases, more and more observations are entrained not only for model validations, but also in the case selections and the constructions of model forcing data.

For configuring LES model runs, initial and boundary conditions are required, together with atmospheric properties (e.g., cloud boundaries, liquid water path [LWP]) at regular intervals for validation. Observations of these initial and boundary conditions, and the validation data, need to be at spatial and temporal scales relevant for the planned LES run. A suitable framework developed by a set of LES and observational experts that has all these required fields along with their uncertainty will greatly help to bring the two communities closer. The framework needs to be flexible to incorporate different LES codes and retrieval techniques. Such an effort will foster collaborations between two communities through process-level studies, LES validation efforts, and identifying retrieval techniques suitable for such efforts. While the LASSO framework meets some of these goals, a limitation is that cases, locations, and observational data sets are manually selected by a single team. A community-driven approach in which tools are available to quickly generate forcing data for a wider variety of cases and models and principal investigators (PIs) could contribute LES output in a standardized format as PI data sets would further these goals more broadly.

Observational studies should aim to 1) provide evidence to support the theoretical development of mechanistic understanding from process studies of LES; 2) provide process-oriented statistics such as ensemble behaviors of golden day cases, and prevailing covariance patterns of variables or lead-lag relationships; 3) document detail case classification and establish case libraries for modeling studies; 4) take advantage of OSSE, simulators and tracking algorithms to design the process-oriented measurements with high spatial and temporal resolution at regional or global scales; 5) create new canonical cases with more comprehensive observations that can be used to constrain and validate models.

2.5.2 Instrument Simulators and Observational System Simulation Experiments (OSSE)

The LES modeling community can also perform long-term runs at fixed sites and use instrument simulators to yield a phase space of measurement variables like radar reflectivity, lidar backscatter, etc. Such an effort, together with OSSE, will help guide the operational settings and placement of current sensors and illuminate needs for new sensors more compatible with LES modeling requirements. Identifying the optimal spacing between distributed sites and optimal sampling patterns of airborne, shipborne. and uncrewed aerial system (UAS) platforms, especially during a large multi-agency field campaign, is a primary hindrance to the observational community. An OSSE of all the involved instrumentation based on large-domain LES runs that resolve the primary desired processes to be studied can guide these sampling strategies.

2.5.3 Data Fusion and Assimilation

Atmospheric instrumentation present at the ARM sites is designed to observe aerosol, cloud, dynamic, radiative, and thermodynamic properties. However, these observations cannot be used directly to derive changes of these properties with time due to a single process, as processes occurring at multiple spatial and temporal scales simultaneously affect them. An atmospheric model in a LES setup is specifically designed to capture these different process rates. An online flexible framework for making LES runs using observed soundings, reanalysis-based thermodynamic and dynamic advective tendencies, and terrain could be made available to the community. For example, extending the LASSO user interface so that investigators could run their own simulations, as well as analyzing pre-run simulations, would be valuable. Such a framework would educate the observational community about LES modeling and provide an independent way to verify 1) whether a model simulates the observed atmospheric properties, and 2) potential sources of the discrepancies between the model and observations. With ever-increasing computing power, potentially these comparisons could be made on an online platform, resulting in rapid advancement in improving our understanding of these processes through improved synergy between observations and LES.

Considering the spatial and temporal resolutions of LES, the use of direct data assimilation may be challenging but not impossible. As mentioned, this is an underexplored research area, but can greatly help the synergy with LES and maximize the use of observations, especially ARM high spatial and temporal resolution data. Also, the systematic and routine comparisons between LES output and observations, e.g., the extension of LASSO (Gustafson et al. 2020), the FASTER project (Liu 2019) and the European CloudNet have proven to be an effective approach to improving models, which is a nice example of synergy between observations and modeling.

2.5.4 Machine Learning Approach

Machine learning techniques can also be applied to observations to help identify key components and improve parameterizations for processes of interest. For example, machine learning has been used to predict momentum fluxes from wind-tunnel observations (Ito and Mouri 2021), total kinetic energy (TKE) from sonic anemometers for complex terrain, and autoconversion and accretion rates from in situ probe measurements (Chiu et al. 2021). The same principle can be applied for cloud chamber measurements and the wide range of ARM remote-sensing observations. These research outputs, however, need to be further combined with modeling activities to fully understand the strengths and limitations of predictions, and to evaluate our process-level understanding. Without the last step of coupling between observations and modeling, the synergy will remain incomplete.

2.5.5 Collaboration in Field Campaigns

With ever-increasing computing power making it easier to make LES runs, and decrease in the cost of instrumentation, it is only a matter of time for the two communities to synergistically work together for improving process-level understanding.

It would be great for modelers to get involved with the field campaigns at the proposal stages, especially process LES modelers and parameterization developers for CRMs or global climate models (GCMs). This approach allows rapid generation of realistic case libraries facilitating rapid model evaluation against observations for a diverse range of conditions. The approach also lends itself to serving as a platform for exploring the role of direct data assimilation into LES, which so far is a largely unexplored research area, but was a recurring topic during the workshop. Understanding what role data assimilation can play in LES research and developing methods to perform data assimilation will likely provide numerous opportunities for LES-related research in the coming decade.

3.0 APPENDICES

Appendix A - Agenda

First day – April 25th (Monday)

7:00–7:10 **Welcome from DOE**

7:10–7:20 **Workshop Introduction** - Kyle Pressel, Yunyan Zhang, and Thijs Heus

7:20–9:30 **Plenary Session 1–The History of LES and the LES in ASR**

7:20–7:50 George Matheou *"Large-eddy simulation: historical and future perspectives"*

7:50–8:20 David Mechem *"LES in ARM and ASR: From GEWEX to LASSO"*

8:20–9:30 Discussion led by Thijs Heus, George Matheou, and David Mechem

9:30–11:30 **Joint Poster Session 1: History of LES and LES in ASR + Process Science (on Slack)**

11:30–14:00 **Plenary Session 2–Process Science**

11:30–12:00 Mikael Witte *"Studying Process with LES: A Bridge Between Micro and Synoptic Scales"*

12:00–12:30 Katia Lamer

12:30–14:00 Discussion Led by Yunyan Zhang, Mikael Witte, and Katia Lamer

14:00 **Adjourn** for the First Day

Second day – April 26th (Tuesday)

7:00–9:30 **Plenary Session 3–LES Model Physics**

7:00–7:30 Katie Lundquist *"Multiscale atmospheric modeling from global and mesoscales to large-eddy simulation"*

7:30–8:00 Laura Fierce *"Particle-based representations of microphysics: lessons from aerosol science and engineering"*

8:00–9:30 Discussion Led by Kyle Pressel, Katie Lundquist, Laura Fierce

9:30–11:30 **Joint Poster Session 2: LES Model Physics + LES Development (on Slack)**

11:30–14:00 **Plenary Session 4–LES Development**

11:30–12:00 Chiel van Heerwaarden *"Dilemmas in LES Development: How to build the next-generation tools with this community?"*

12:00–14:00 Discussion Led by Kyle Pressel and Chiel van Heerwaarden

14:00 **Adjourn** for the Second Day

Appendix B - Participants

An initial list of invitees was composed by the organizers, after which the invitees could suggest further nominations, with an explicit preference for early career scientists. While any group of limited size will have omissions in invitation and attendance, there was reasonable representation during the meeting across national laboratories and academia, US and abroad, career stage and gender, and professional specialty.

Workshop Registrants

Peter Blossey, *University of Washington*

Peter Bogenschutz, *Lawrence Livermore National Laboratory*

Jingyi Chen, *Pacific Northwest National Laboratory*

Maria Chinita, *Jet Propulsion Laboratory*

Christine Chiu, *Colorado State University*

Tina Chow, *University of California, Berkeley*

Patrick Chuang, *University of California-Santa Cruz*

Jennifer Comstock, *Pacific Northwest National Laboratory*

Alex Connolly, *Columbia University*

Fleur Couvreux, *CNRM, Meteo-France and CNRS*

Shannon Davis, *Wind Energy Technologies Office, US Department of Energy*

Jeramy Dedrick, *Scripps Institution of Oceanography*

Jiwen Fan, *Pacific Northwest National Laboratory*

Jerome Fast, *Pacific Northwest National Laboratory*

Graham Feingold, *NOAA*

Daniel Feldman, *Lawrence Berkeley National Laboratory*

Laura Fierce, *Pacific Northwest National Laboratory*

Ann Fridlind, *NASA GISS*

Gerald Geernaert, *Department of Energy*

Virendra Ghate, *Argonne National Laboratory*

William Gustafson, *Pacific Northwest National Laboratory*

Thijs Heus, *Cleveland State University*

Adrian Hill, *The UK Met Office*

Anna Jaruga, *Caltech*

Colleen Kaul, *Pacific Northwest National Laboratory*

Jan Kazil, *NOAA*

Daniel Kirshbaum, *McGill University*

Stephen Klein, *Lawrence Livermore National Laboratory*

Pavlos Kollias, *Stony Brook University/Brookhaven National Laboratory*

Branko Kosovic, *National Center for Atmospheric Research*

Steven Krueger, *University of Utah*

Chongai Kuang, *Brookhaven National Laboratory*

Zhiming Kuang, *Harvard University*

Marcin Kurowski, *Jet Propulsion Laboratory*

Katia Lamer, *Brookhaven National Laboratory*

Neil Lareau, *University of Nevada, Reno*

Vincent Larson, *University of Wisconsin, Milwaukee*

Heping Liu, *Washington State University, Pullman*

Yangang Liu, *Brookhaven National Laboratory*

Katherine Lundquist, *Lawrence Livermore National Laboratory*

Georgios Matheou, *University of Connecticut*

David Mechem, *University of Kansas*

Jeff Mirocha, *Lawrence Livermore National Laboratory*

Hugh Morrison, *National Center for Atmospheric Research*

Mikhail Ovchinnikov, *Pacific Northwest National Laboratory*

Kyle G. Pressel, *Pacific Northwest National Laboratory*

Mike Pritchard, *University of California, Irvine*

David Richter, *University of Notre Dame*

David Romps, *Lawrence Berkeley National Laboratory*

Lynn Russell, *Scripps Institute of Oceanography, University of California, San Diego*

Koichi Sakaguchi, *Pacific Northwest National Laboratory*

Shawn Serbin, *Brookhaven National Laboratory*

Sara Shamekh, *Columbia University*

Raymond Shaw, *Michigan Technological University*

Jacob Shpund, *Pacific Northwest National Laboratory*

Jason Simon, *Duke University*

Yang Tian, *National Center for Atmospheric Research*

Dave Turner, *NOAA / Global Systems Laboratory*

Chiel van Heerwaarden, *Wageningen University*

Marcus van Lier-Walqui, *Columbia University*

Bart van Stratum, *Wageningen University & Research*

Adam Varble, *Pacific Northwest National Laboratory*

Andrew Vogelmann, *Brookhaven National Laboratory*

Hailong Wang, *Pacific Northwest National Laboratory*

Dié Wang, *Brookhaven National Laboratory*

Adam Wise, *University of California, Berkeley*

Mikael Witte, *Naval Postgraduate School*

Robert Wood, *University of Washington*

Shaocheng Xie, *Lawrence Livermore National Laboratory*

Takanobu Yamaguchi, *CIRES, University of Colorado / NOAA CSL*

Fan Yang, *Brookhaven National Laboratory*

Mónica Zamora Zapata, *Universidad de Chile*

Yunyan Zhang, *Lawrence Livermore National Laboratory*

Xue Zheng, *Lawrence Livermore National Laboratory*

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Appendix D - Acronyms and Abbreviations

1D	one-dimensional
2D	two-dimensional
3D	three-dimensional
AAF	ARM Aerial Facility
AOS	Aerosol Observing System
APU	accelerated processor unit
ARM	Atmospheric Radiation Measurement
ASR	Atmospheric System Research
ASTEX	Atlantic Stratocumulus Transition Experiment
ATEX	Atlantic Trade-Wind Experiment
BER	Biological and Environmental Research
BOMEX	Barbados Oceanographic and Meteorological Experiment
CCN	cloud condensation nuclei
CFL	Courant-Friedrichs-Lewy
CPU	central processing unit
CRM	cloud-resolving model
DOE	U.S. Department of Energy
DOI	digital object identifier
DYCOMS	Dynamics and Chemistry of Marine Stratocumulus
E3SM	Energy Exascale Earth System Model
ESM	Earth system model
GCM	global climate model
GCSS	GEWEX Cloud System Study
GEWEX	Global Energy and Water Exchanges
GLAFO	GEWEX Land-Atmosphere Feedback Observatory
GPCI	GEWEX/WGNE Pacific Cross-section Intercomparison
GPU	graphics processing unit

HI-SCALE	Holistic Interactions of Shallow Clouds, Aerosols, and Land-Ecosystems
HPC	high-performance computing
IN	ice nuclei
IO	input/output
ISDAC	Indirect and Semi-Direct Aerosol Campaign
LAFE	Land-Atmosphere Feedback Experiment
LASSO	LES ARM Symbiotic Simulation and Observation Activity
LES	large-eddy simulation
LSM	land surface model
LWP	liquid water path
MAGIC	Marine ARM GPCI Investigation of Clouds
ModEx	model-experiment
MPI	message passing interface
NWP	numerical weather prediction
OSSE	Observational System Simulation Experiment
PBL	planetary boundary layer
PI	principal investigator
PSD	particle size distribution
RACORO	Routine AAF Clouds with Low Optical Water Depths (CLOWD) Optical Radiative Observations
RT	radiative transfer
SAIL	Surface Atmosphere Integrated Field Laboratory
SBM	spectral bin microphysics
SD	superdroplet
SFS	subfilter scale
SGP	Southern Great Plains
TKE	total kinetic energy
UAS	uncrewed aerial system
WGNE	Working Group on Numerical Experimentation
WRF	Weather Research and Forecasting

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