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

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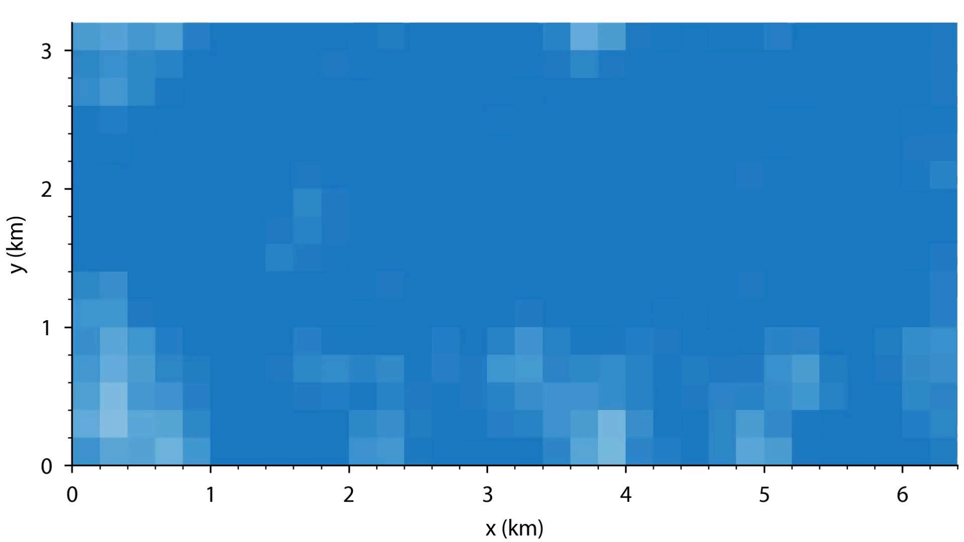
Workshop Background

- Explicit representation of three-dimensional turbulence makes LES ideal for process studies
- LES is applied with increasing complexity for representing various physical processes
- Process-oriented LES studies support DOE's and ASR's missions
- Broader applications of LES grow with the computational power/resources

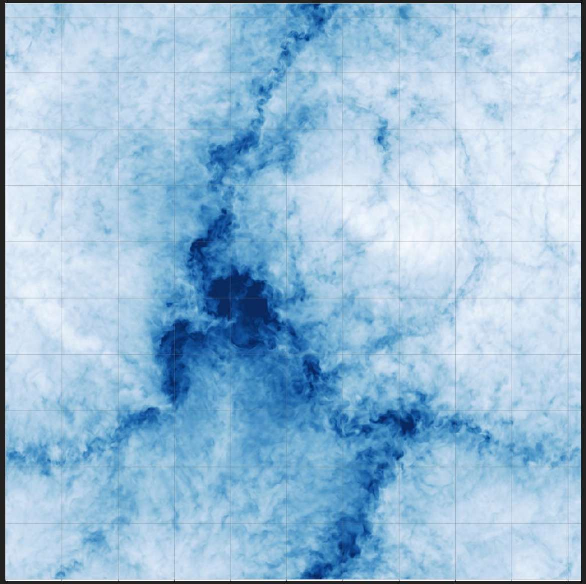


ARM-SGP LES with 1970s - 2020s-style grid spacing (200m - 6m; courtesy Chiel van Heerwaarden)

Motivation, Participants, and Unifying Questions

- Goal: Discuss the science that LES can/will drive over the next decade
- 70 participants from 40 institutions
- Inputs from observationalists, LES developers, and process scientists
- The workshop sought to answer five themes:

1. *What are the key opportunities*
2. *Limitations in physical process representation in LES*
3. *Implementation and infrastructure limitations*
4. *Observational needs*
5. *Opportunities for synergy between Observations and LES*



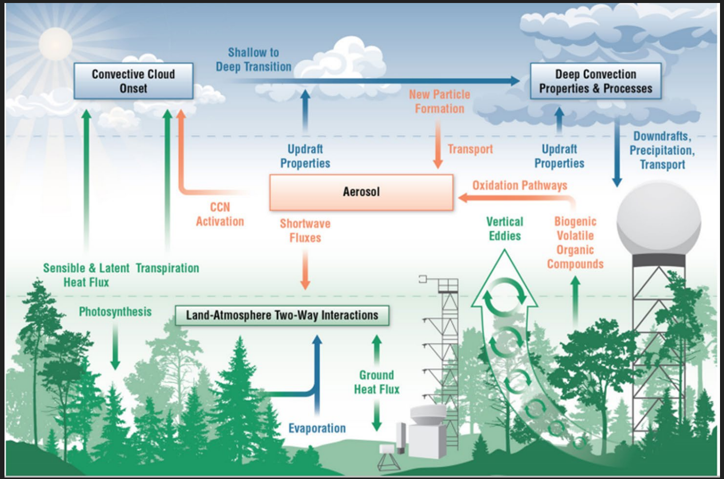
What are the opportunities for LES-related research for atmospheric aerosol, cloud, and precipitation process studies over the next 5 to 10 years?

Opportunities are largely determined by how increasing HPC resources will be leveraged.

- Routine LES
  - Large ensembles of LES enabling statically robust process studies
  - Uncertainty quantification
  - Generation of LES-based Machine Learning (ML) training datasets
  - Fine-scale modeling component of Model-Observation System-Experiment Paradigm (ModEx) based Studies and Operational System Simulation Experiments (OSSEs)
- Increasing computational complexity of individual LES
  - Higher resolution - statistically grid converged LES
  - Larger domain realistic LES with non-periodic boundary conditions, data assimilation, heterogeneous surface boundary conditions
  - Detailed process representations - 3D radiative transfer, advanced microphysics, aerosol-cloud-chemistry interactions.

Blender rendered cumulus;
courtesy Roel Neggers

What physical process representations in LES will limit research progress over the next 10 years?



Courtesy of SEUS science team

- Physical Complexity == Computational Cost
- Many subprocesses are borrowed from coarser models, and not always valid at LES scale, for instance:
  - One-Dimensional radiation
  - Simple Monin-Obukhov-based surface schemes
- Process typically absent
  - Complex topography, urban, biological LAI
  - Chemistry and Aerosol processes
- Sub-filter scale (SFS) modeling need improvement,
  - especially for non-linear SFS processes (i.e. condensation or chemical reactions) and under stable stratification

Memory bound GPU simulations offer an opportunity to seek computationally intensive solutions

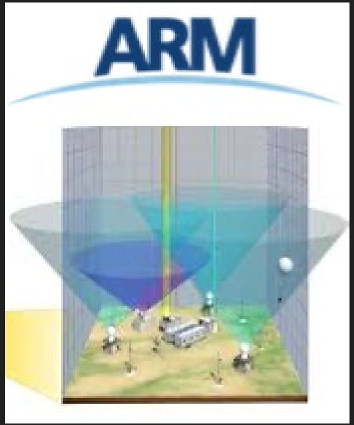
What aspects of current LES implementations will limit research progress over the next 10 years?

- Next-gen supercomputers are all GPU-based; few developers can code for complex modern architectures
    - Using modern programming languages and frameworks would widen the pool of developers
- Rethink tuning of IO, standardizing datasets, selection of online calculated stats, cloud-based postprocessing
- Best OpenScience practices
    - (code management, continuous integration, documentation)
- Compressible or incompressible governing equations?
- Revisit existing LES benchmarks to generate a benchmark at modern resolution/process complexity
    - New benchmarks needed, e.g. focus on aerosol cloud interactions
- A delicate balance between community models and small-group-LES

What kind of observations would be useful in improving and further validating LES?

In the next decade or so, we should strive to improve our observational capability to

- Bridge the scale gap between measurement resolution and the native scale of key processes
- Increase the spatial representativeness of variability in vertical motions, heterogeneities, and temporal evolution.



To validate and improve LES, these data are specifically needed:

- Continuous vertical profiling of T/Q, U/V/W, turbulent fluxes, cloud water/ice partitions, aerosols, CCN/IN and precipitation
- Spatially distributed and co-located measurements over heterogeneous land covers
- Canonical climate/cloud regimes to build up statistics from ensembles as well as measurements into extreme regimes to help explore the climate sensitivities
- Detailed morphology statistics of individual cloud and precipitation clusters and their interactions or the Lagrangian evolution of a cluster’s life cycle
- Cloud chamber experiments on microphysical processes and their associated specifically-designed LES simulations.

What opportunities exist for improved synergy between observations and LES in studies of the atmosphere, and what are the challenges in doing so?

- Instrument simulators and OSSEs
  - Apple-to-apple comparisons
  - Guidance to observational sampling strategies

- Leveraging machine learning approaches based on observational data to guide LES process-representation development.

- Observationally constrained case bundles, including:
  - Forcing files
  - Observational diagnostics and statistics

- Model developers involvement in field campaign planning (e.g., SEUS)

Conclusions

- LES is getting more complex yet more accessible to a larger public
- Synergy with observations a huge potential
- Machine Learning plays a crucial role in improving LES - and LES in improving ML
- Need to revisit physics representation directly from the LES scales
- GPU computing generates more opportunities and more challenges
- An organized community and community model with support will be key