1. **Influences of the Boundary Layer Flow on Vegetation-Air Exchanges of Energy, Water and Carbon Dioxide**

Xuhui Lee (Yale University) and Edward Patton (NCAR)

- Summarize your projects and its scientific objectives for the next 3-5 years

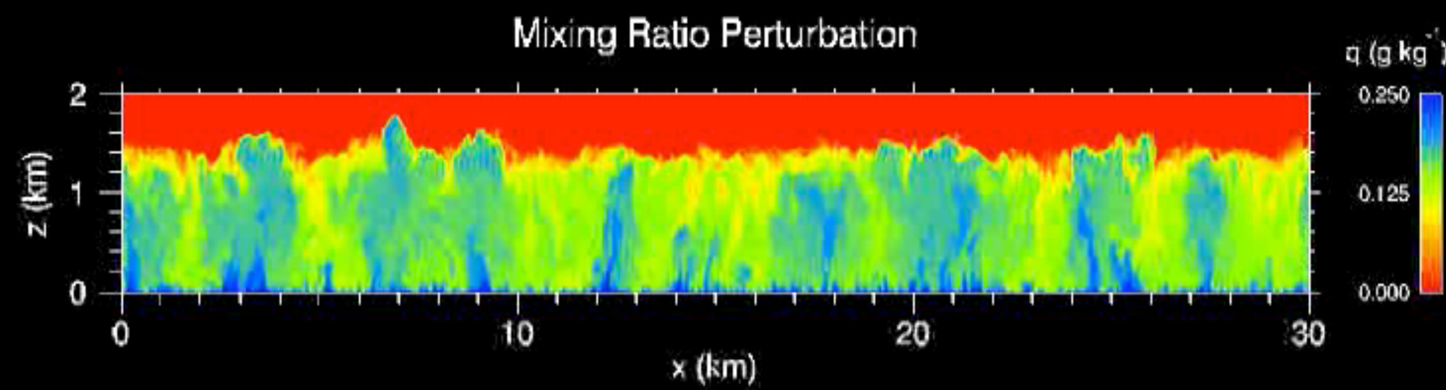
The objective of this project is to establish a mechanistic understanding of the interplay between flow heterogeneity in the atmospheric boundary layer (ABL), land surface heterogeneity, and vegetation-air exchange of energy, water and CO_2.

The project will investigate mechanisms by which mesoscale motions in the ABL influence vegetation-air exchange.

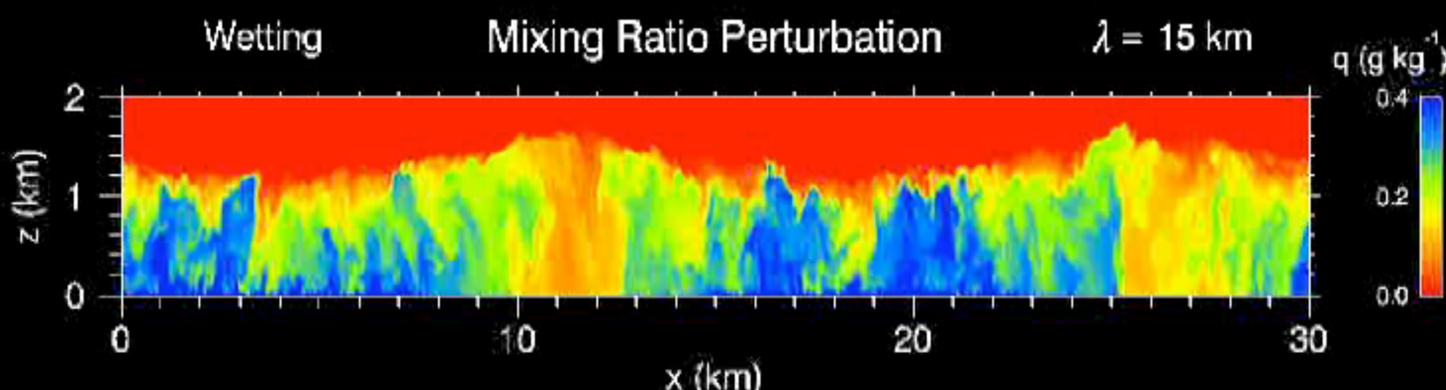
It will also quantify the influence of heterogeneity on predictions by 1D column models used in regional and global scale climate models.

It is hypothesized that two important ABL processes entrainment and flow heterogeneity cause biases in the observation and model estimates of vegetation-air exchange and that the degree of bias is different for active (heat and water) and passive (CO_2) scalars.

Horizontally Homogeneous

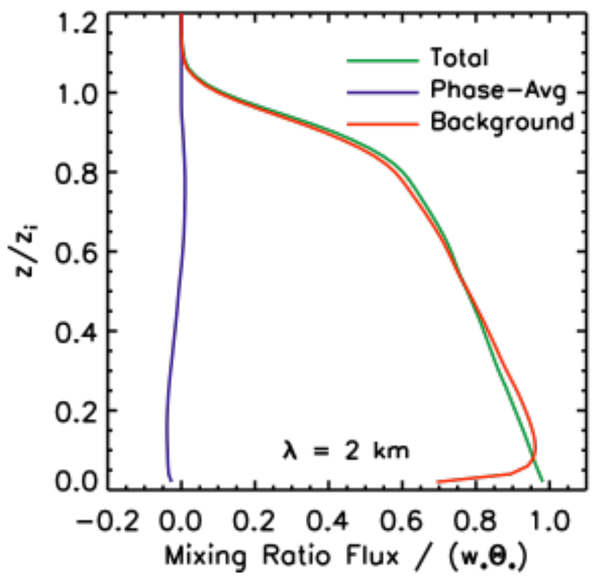


Mesoscale Horizontal Heterogeneity $\lambda/z_i \sim 9$

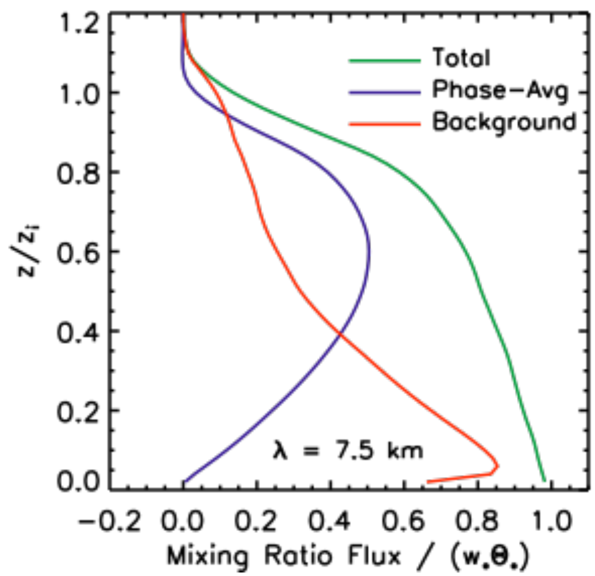


Vertical Moisture Fluxes - Influence on measurements

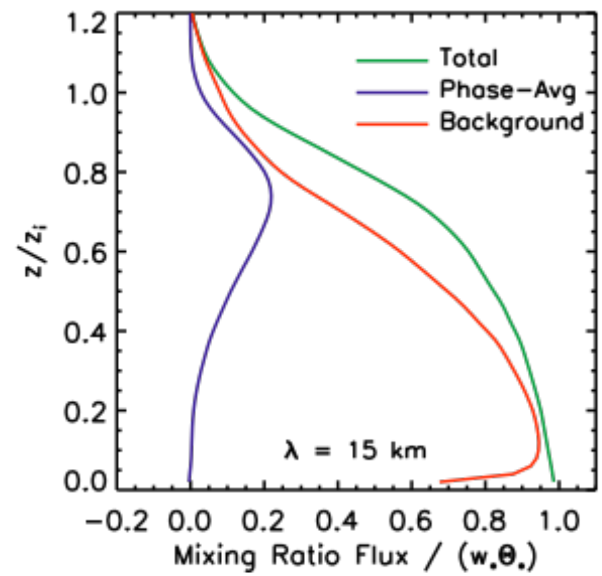
$\lambda / z_i \approx 1$



$\lambda / z_i \approx 4$



$\lambda / z_i \approx 9$



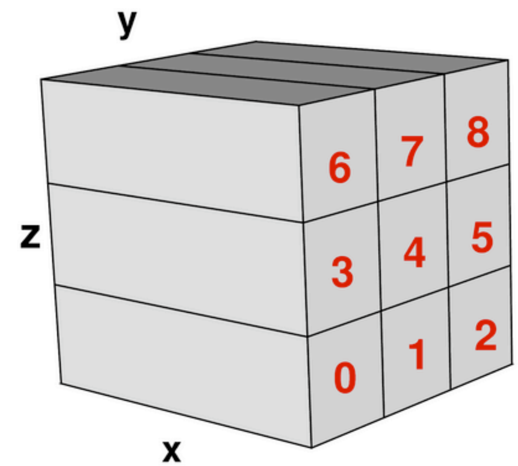
MASSIVELY PARALLEL ALGORITHM FOR BOUSSINESQ BOUNDARY LAYERS

Algorithm Constraints:

- Utilize 2-D domain decomposition

- Employ a mixed pseudospectral finite-difference scheme

- Incompressible flow must solve $\nabla^2 p = s$



Highlights:

- Employ *local* MPI matrix transposes to evaluate derivatives and solve for the pressure:
  $f(x,\, y_s\!:\!y_e,\, z_s\!:\!z_e) \;\Leftrightarrow\; f^T(y, x_s\!:\!x_e, z_s\!:\!z_e)$
  $\hat{s}(k_y, k_{xs}\!:\!k_{xe}, z_s\!:\!z_e) \;\Leftrightarrow\; \hat{s}^T(z, k_{xs}\!:\!k_{xe}, k_{ys}\!:\!k_{ye})$

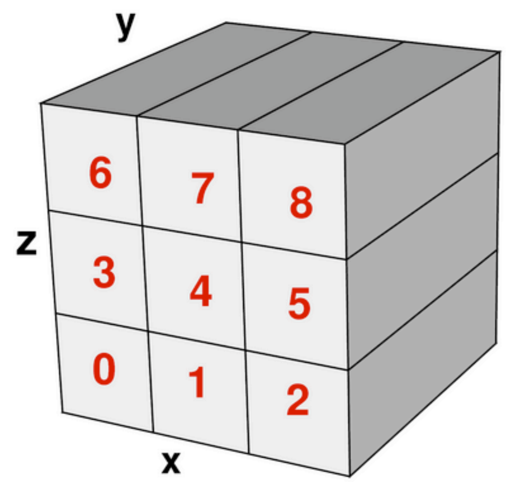
- No ALLTOALLV global communication,
  use SENDRECV

- Use MPI I/O, single large direct-access like file

MASSIVELY PARALLEL ALGORITHM FOR BOUSSINESQ BOUNDARY LAYERS

Algorithm Constraints:

- Utilize 2-D domain decomposition
- Employ a mixed pseudospectral finite-difference scheme
- Incompressible flow must solve $\nabla^2 p = s$



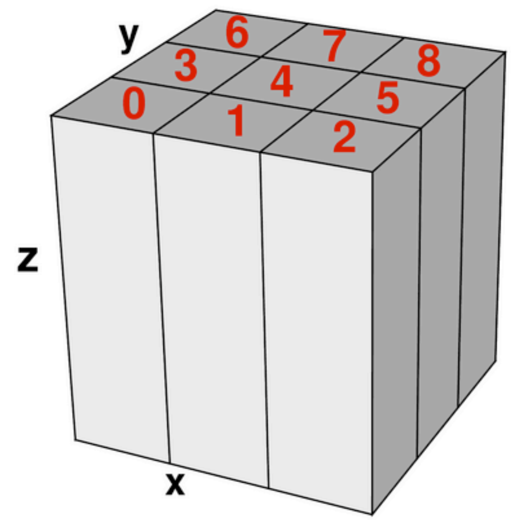
Highlights:

- Employ *local* MPI matrix transposes to evaluate derivatives and solve for the pressure:
  $f(x,\, y_s\!:\!y_e,\, z_s\!:\!z_e) \;\Leftrightarrow\; f^T(y, x_s\!:\!x_e, z_s\!:\!z_e)$
  $\hat{s}(k_y, k_{xs}\!:\!k_{xe}, z_s\!:\!z_e) \;\Leftrightarrow\; \hat{s}^T(z, k_{xs}\!:\!k_{xe}, k_{ys}\!:\!k_{ye})$
- No ALLTOALLV global communication,
  use SENDRECV
- Use MPI I/O, single large direct-access like file

MASSIVELY PARALLEL ALGORITHM FOR BOUSSINESQ BOUNDARY LAYERS

Algorithm Constraints:

- Utilize 2-D domain decomposition
- Employ a mixed pseudospectral finite-difference scheme
- Incompressible flow must solve $\nabla^2 p = s$



Highlights:

- Employ *local* MPI matrix transposes to evaluate derivatives and solve for the pressure:
  $f(x,\, y_s\!:\!y_e,\, z_s\!:\!z_e) \;\Leftrightarrow\; f^T(y, x_s\!:\!x_e, z_s\!:\!z_e)$
  $\hat{s}(k_y, k_{xs}\!:\!k_{xe}, z_s\!:\!z_e) \;\Leftrightarrow\; \hat{s}^T(z, k_{xs}\!:\!k_{xe}, k_{ys}\!:\!k_{ye})$
- No ALLTOALLV global communication,
  use SENDRECV
- Use MPI I/O, single large direct-access like file

NCAR LES on Franklin

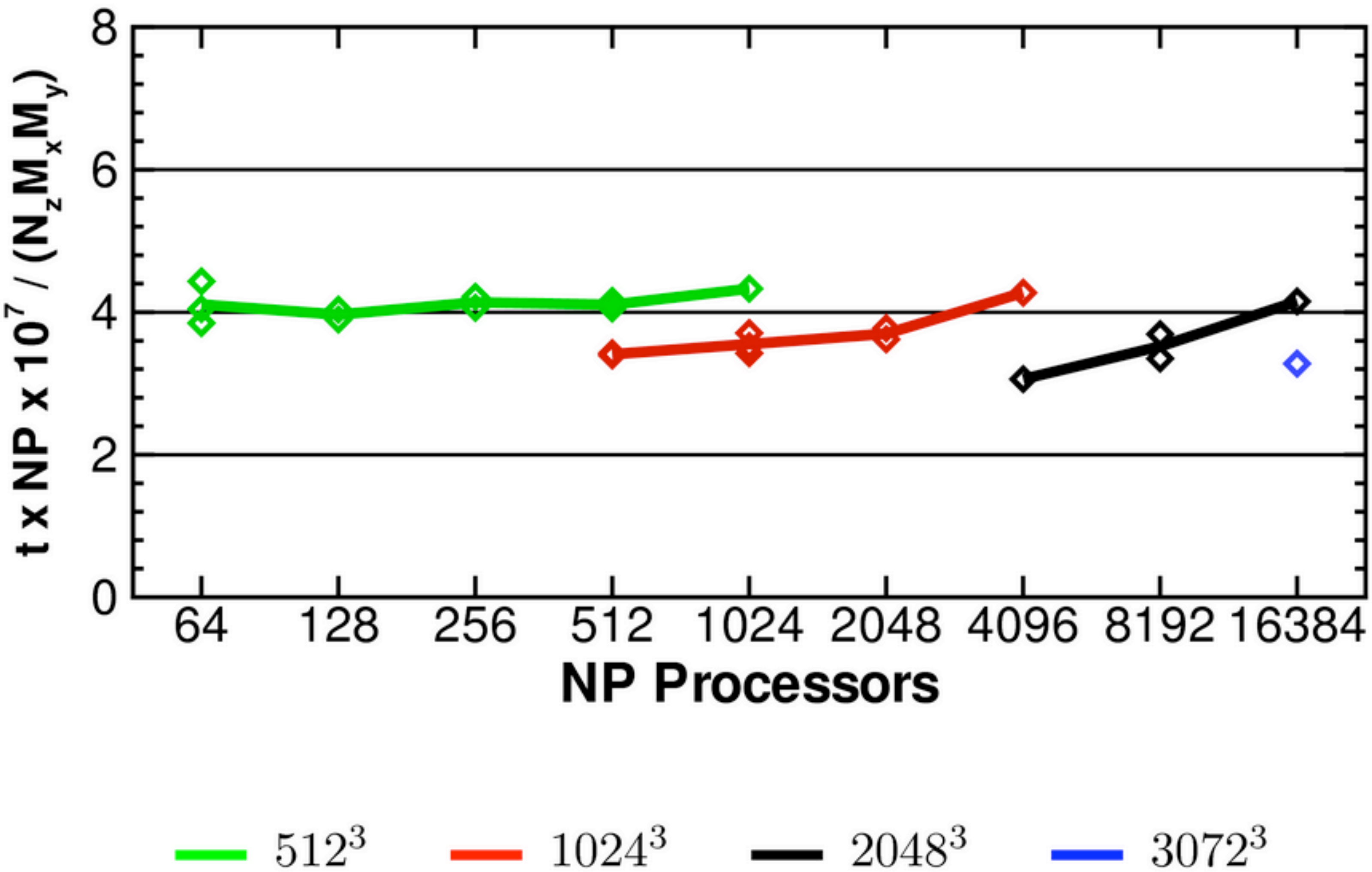
- 2048 x 2048 x 2048 grid points
- 8192 CPUs
- 5120 x 5120 x 2048 m^3
- 2.5 x 2.5 x 1 m^3 resolution
- 36 hours wallclock time – about 600s simulated time

- 216 wallclock hours (9 days) for 1 hour simulated time

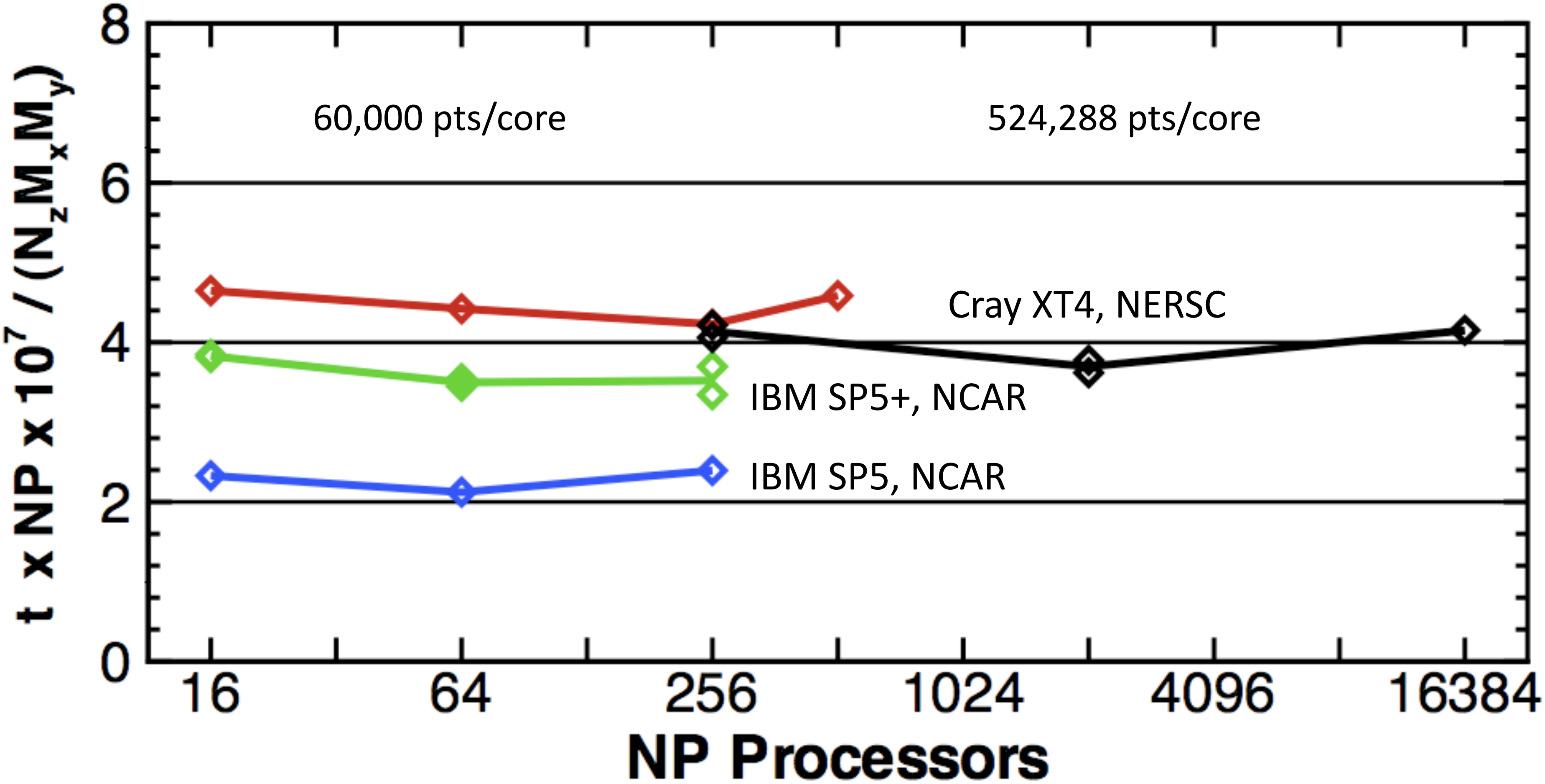
SCALING OF PARALLEL PSEUDOSPECTRAL ALGORITHM WITH 2-D DOMAIN DECOMPOSITION

Cray XT4, NERSC

Strong scaling

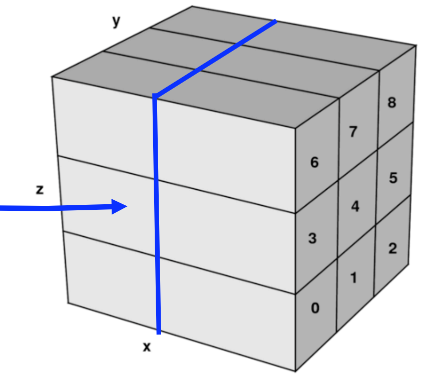


Weak scaling

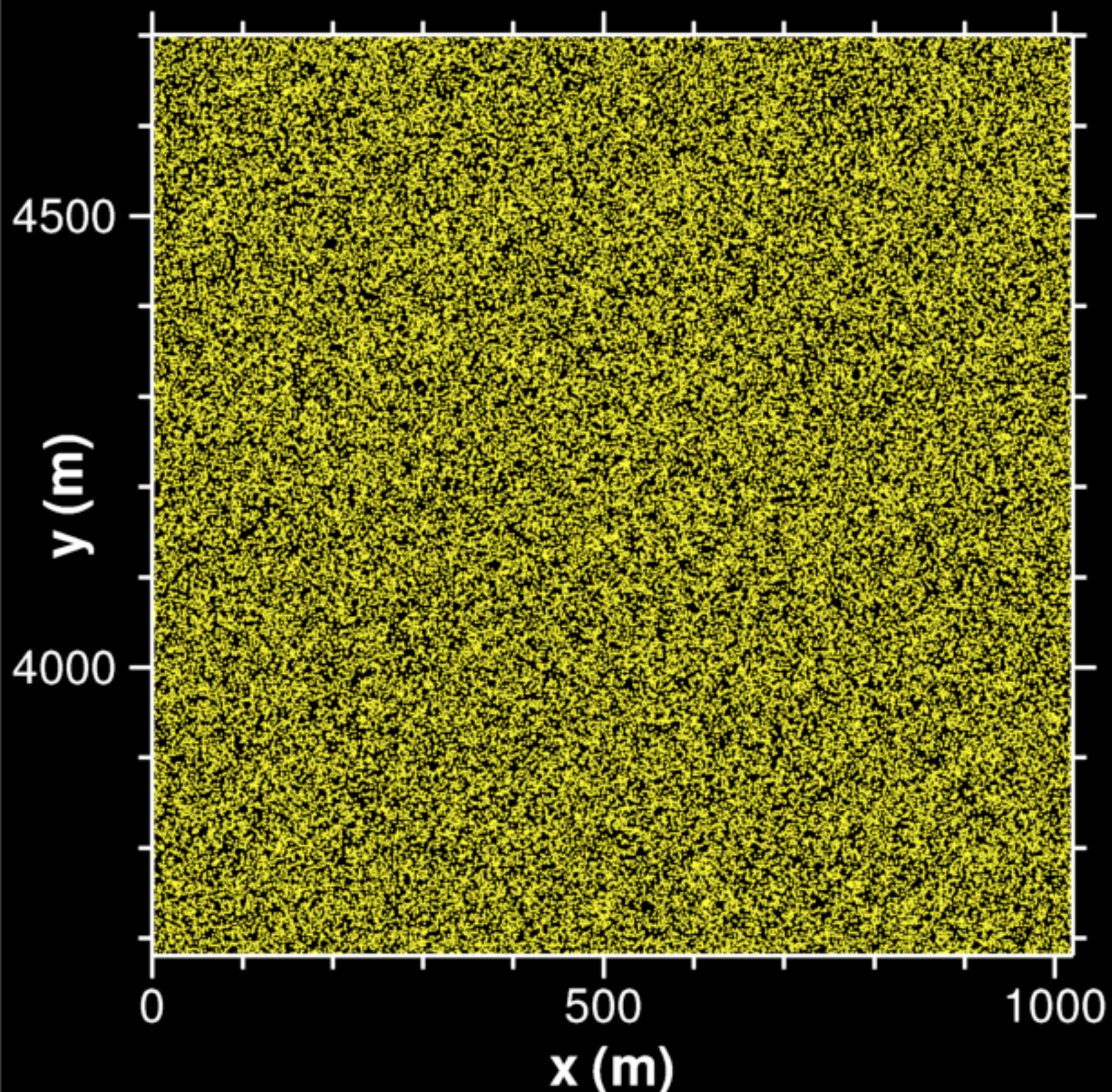


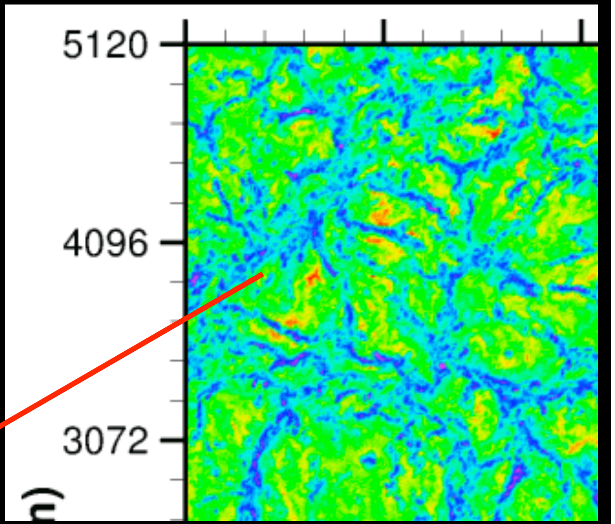
NCAR LES on Franklin

- 3D volumes of five to six REAL(KIND=8) variables stored in IEEE binary in a single file using MPI I/O (~ 400 GB per volume).
- Vertical profiles of horizontally-averaged statistics calculated every time step and stored in 'history' files.
- 2D instantaneous slices saved for visualizations at specified intervals using MPI I/O.
  - Complications when saving planes of data spanning across the MPI breakdown; every CPU must write only a small piece.



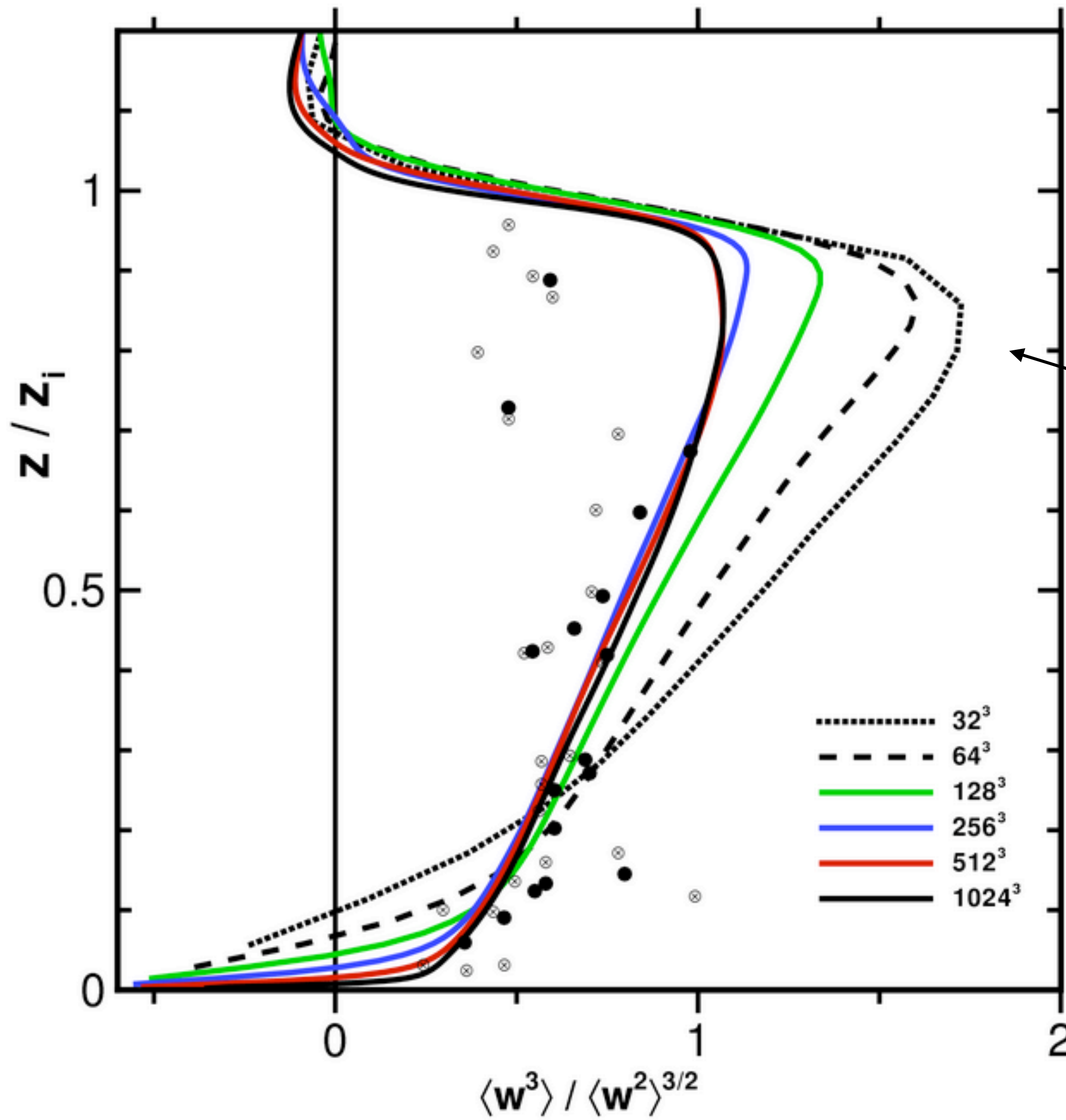
PARTICLE TRACKING IN X-Y PLANE **1024^3** SIMULATION





Dust devil image courtesy NASA

IMPACT OF GRID RESOLUTION ON SKEWNESS



Small scales?
Inversion strength?
SGS model?

1. Impact of vegetation on turbulence over complex terrain: a wind energy perspective

Edward Patton and Peter Sullivan (NCAR)

- Summarize your projects and its scientific objectives for the next 3-5 years

Wind turbines are frequently deployed in regions of undulating topography to take advantage of the expected speed-up of wind as the atmosphere is forced up over the hill.

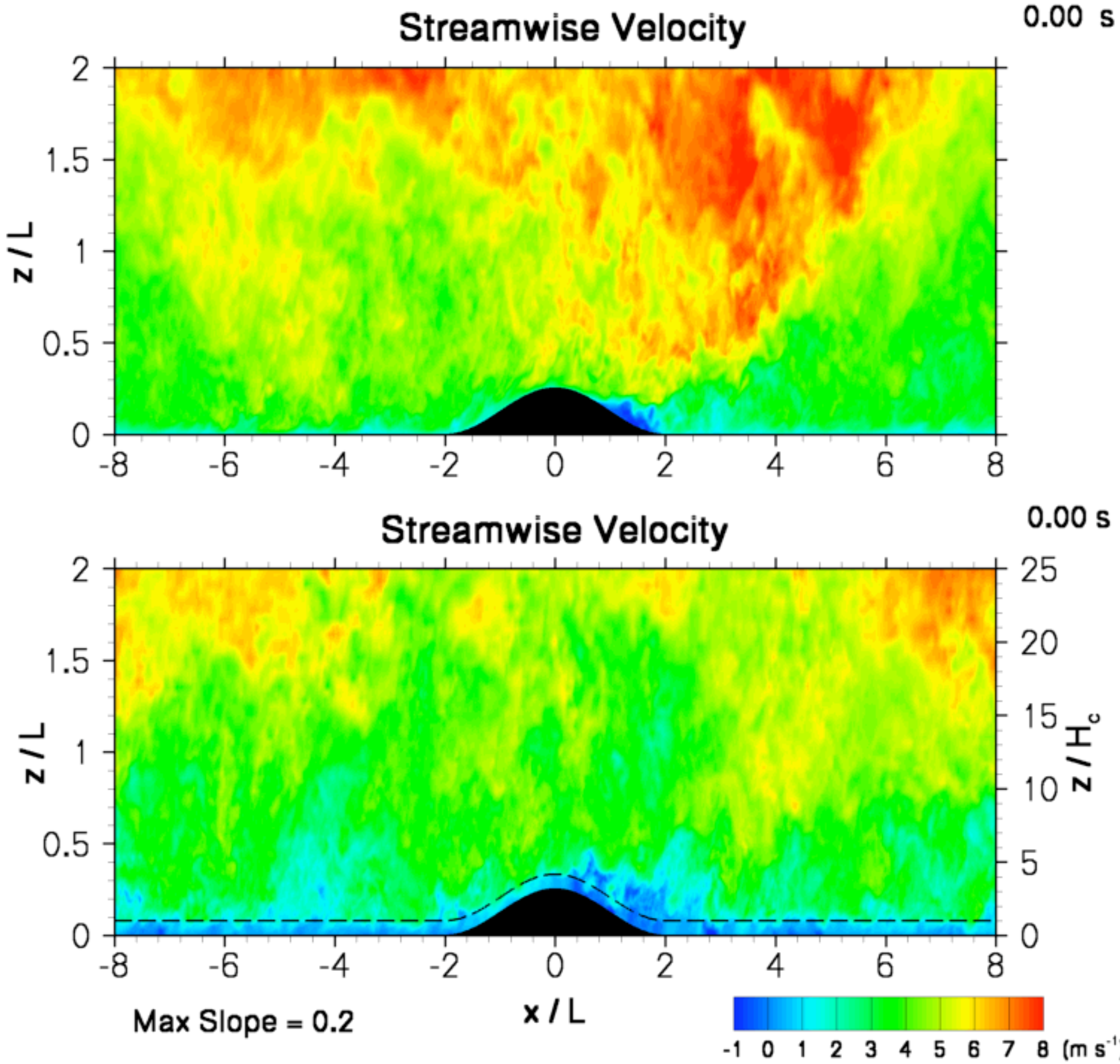
This reasoning is quite simple for an idealized isolated hill in a non-stratified non-vegetated environment, but vegetation and stratification interacts with turbulence in orography in complex ways that are not yet clearly established.

Recently, it has been shown that pressure drag imposed on the flow by the trees can interact with orographically-induced pressure drag in ways that shift the pressure minima downstream of the hill crest making the hill appear more steep to the flow than it otherwise would.

Proper characterization of turbulence in this regime is essential for wind turbine deployment strategy and for turbine design capable to withstand these environments.

We will evaluate turbulence length scales and their variation across stability and hill steepness to guide our understanding of the mechanisms generating the turbulence and its parameterization.

Specified roughness vs. resolved canopy

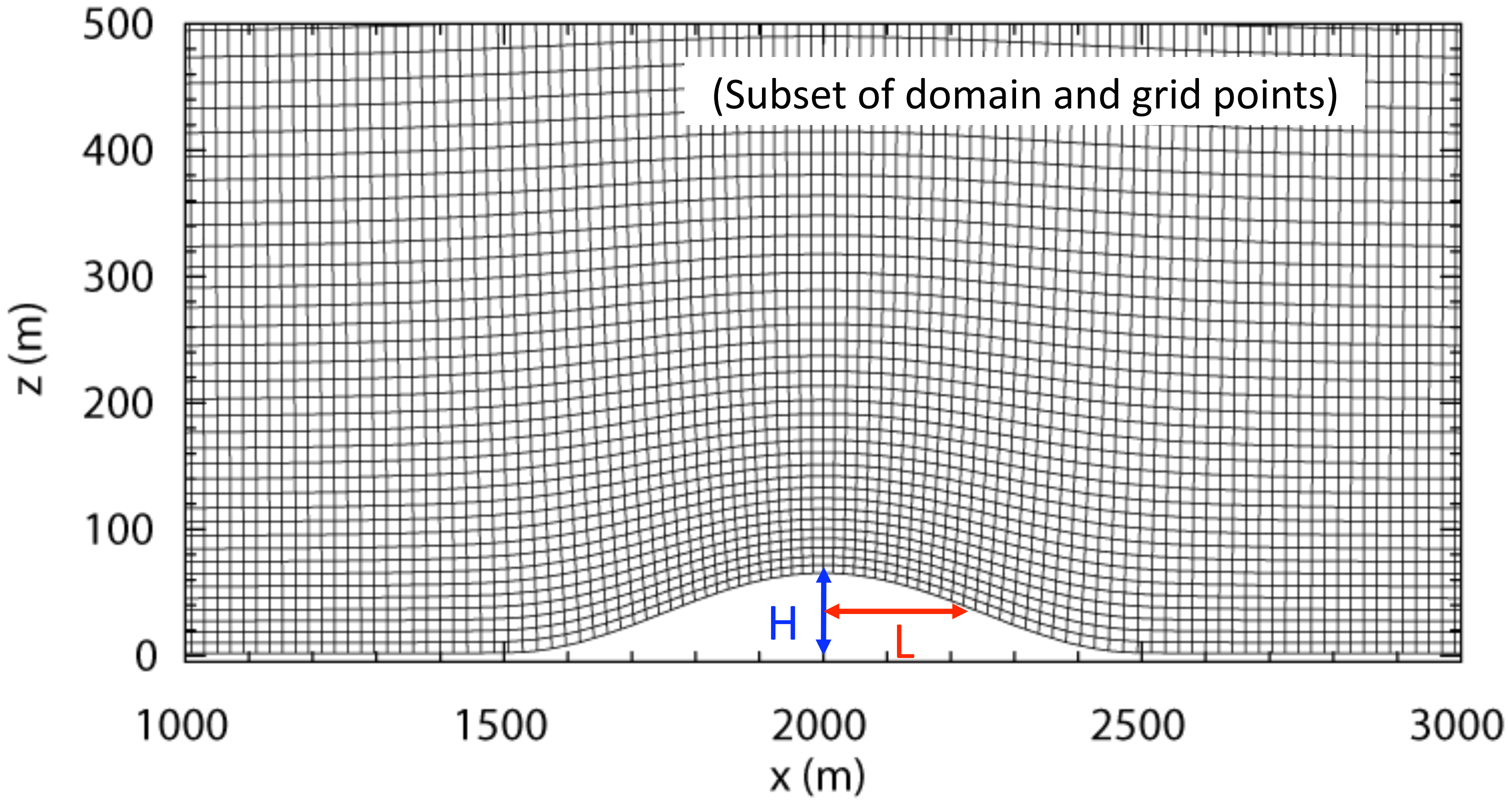


Surface roughness

Neutral stability

Resolved canopy

Schematic Grid Resolving Isolated Hill



- Curvilinear coordinate system (allows for steep terrain)
- Domain
  - 4 km x 1 km x 1.8 km (800 x 200 x 144 grid points)
  - Δx = 5 m
  - Δz = 2 m grid stretching in vertical
- Hill Specifics
  - L = 250 m
  - H / L = 0.25
  - Cosine shape
  - Maximum slope = 0.2

2. Current HPC Requirements

- Architectures:
  - Cray-XT, IBM Power, BlueGene, Linux Cluster, SGI Altix
- Core-hours:
  - ~1 x10^6 core-hrs
  - Typical run:
    - 64-4096 cores
    - 12-600 Wallclock hours
- Memory
  - 2 GB
- Data read/written:
  - Per run: 4-2000 GB
  - Checkpoint files: 2-500 GB
- Necessary software, services or infrastructure:
  - FORTRAN90
  - MPI, MPI-I/O
- Current primary codes and their methods or algorithms
  - NCAR LES, FFTPACK
- Known limitations/obstacles/bottlenecks
  - Node up-time
  - I/O issues

3. HPC Usage and Methods for the Next 3-5 Years

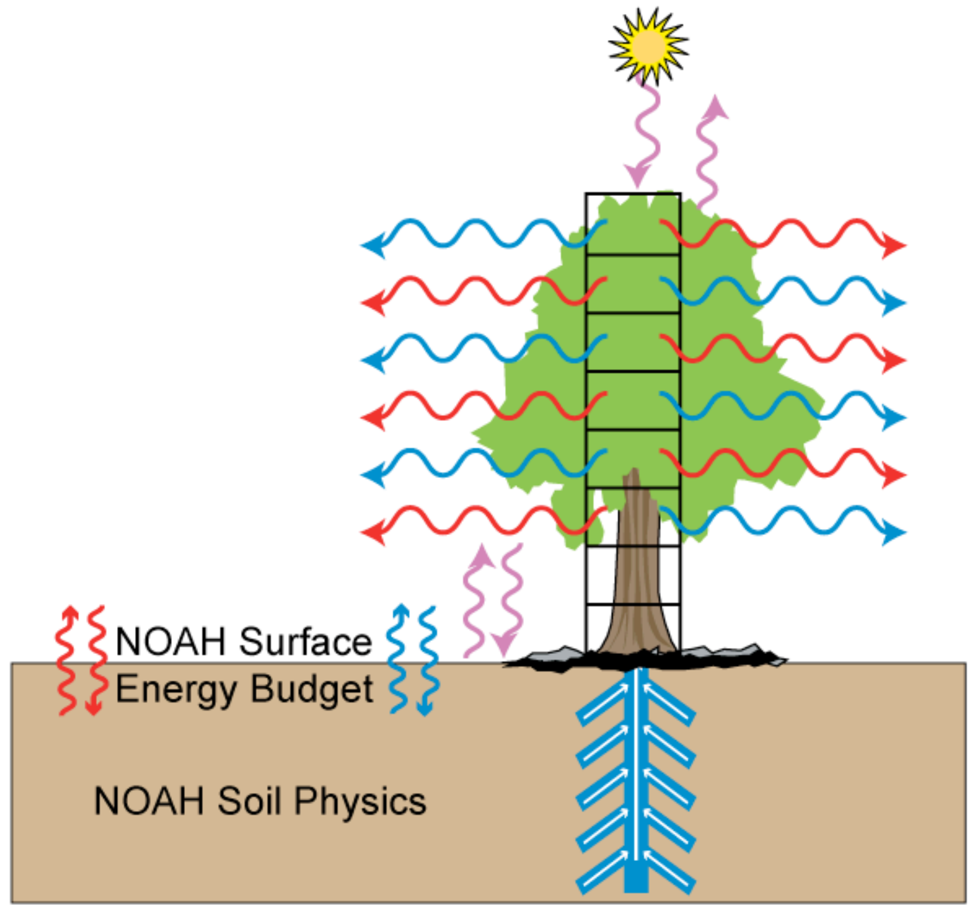
- Upcoming changes to codes/methods/approaches
  - 3D hills
  - Time-dependent grids (3D water waves)
  - Clouds
  - Chemistry (50+ additional scalars)
  - Coupled canopy source/sinks
  - 3D radiation, ray tracing?

- Changes to Compute/memory load
  - Increase according the the problem type

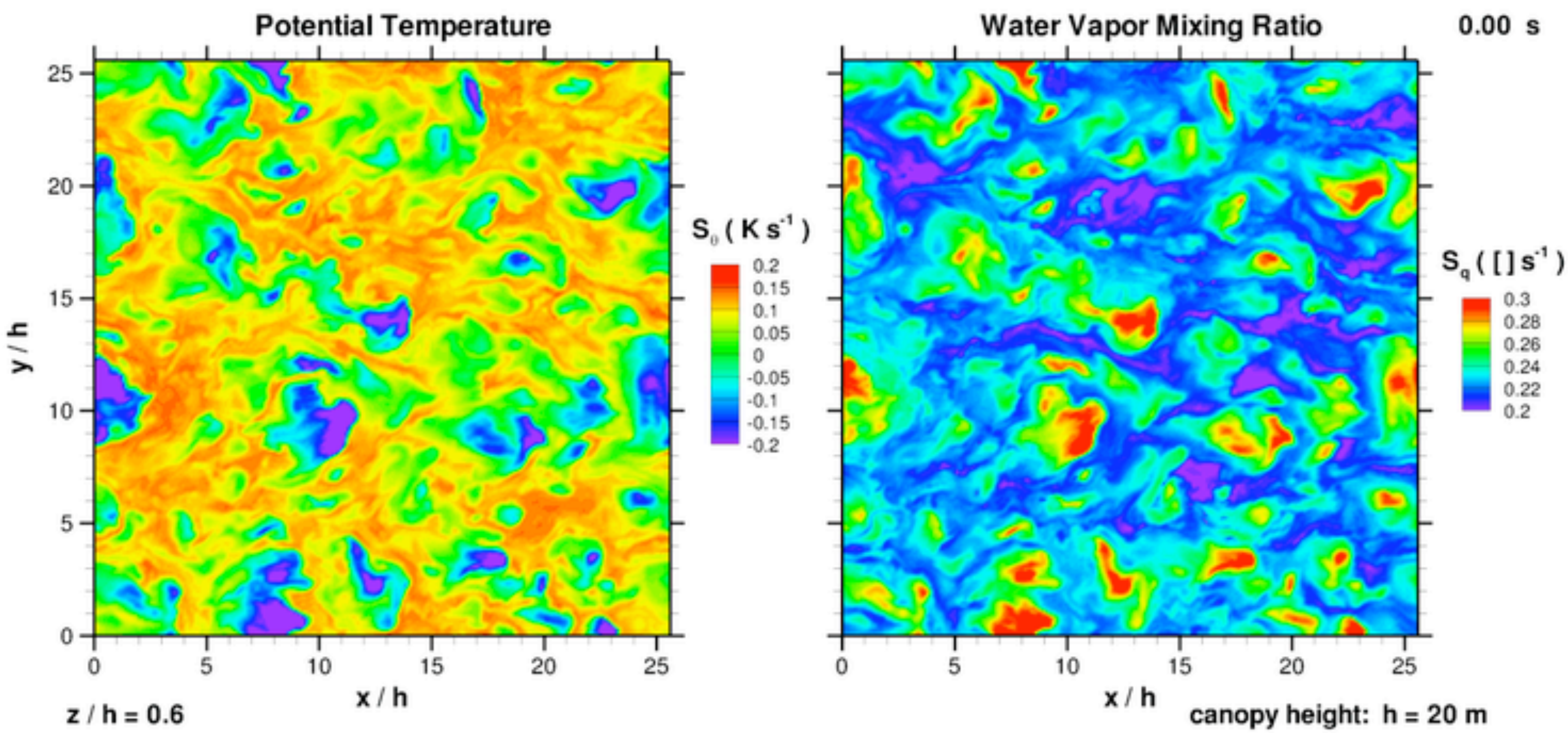
- Changes to Data read/written
  - Again, Increase according the the problem type

Canopy-resolving land-surface model

- using externally provided:
  - winds, temperature, humidity CO_2 and radiation
- the model predicts a profile of canopy
  - leaf temperature
  - radiation absorption
  - sensible heat flux
  - latent heat flux
  - CO_2 uptake



Time- and spatially-dependent vegetation source/sink distributions



4. Summary

- What new science results might be afforded by improvements in NERSC computing hardware, software and services?

- Recommendations on NERSC architecture, system configuration and the associated service requirements needed for your science
  - Reliability
  - Help with deciding appropriate programming model for upcoming architectures
  - Homogeneous architecture (consistent across the machine)