Los Alamos
NATIONAL LABORATORY

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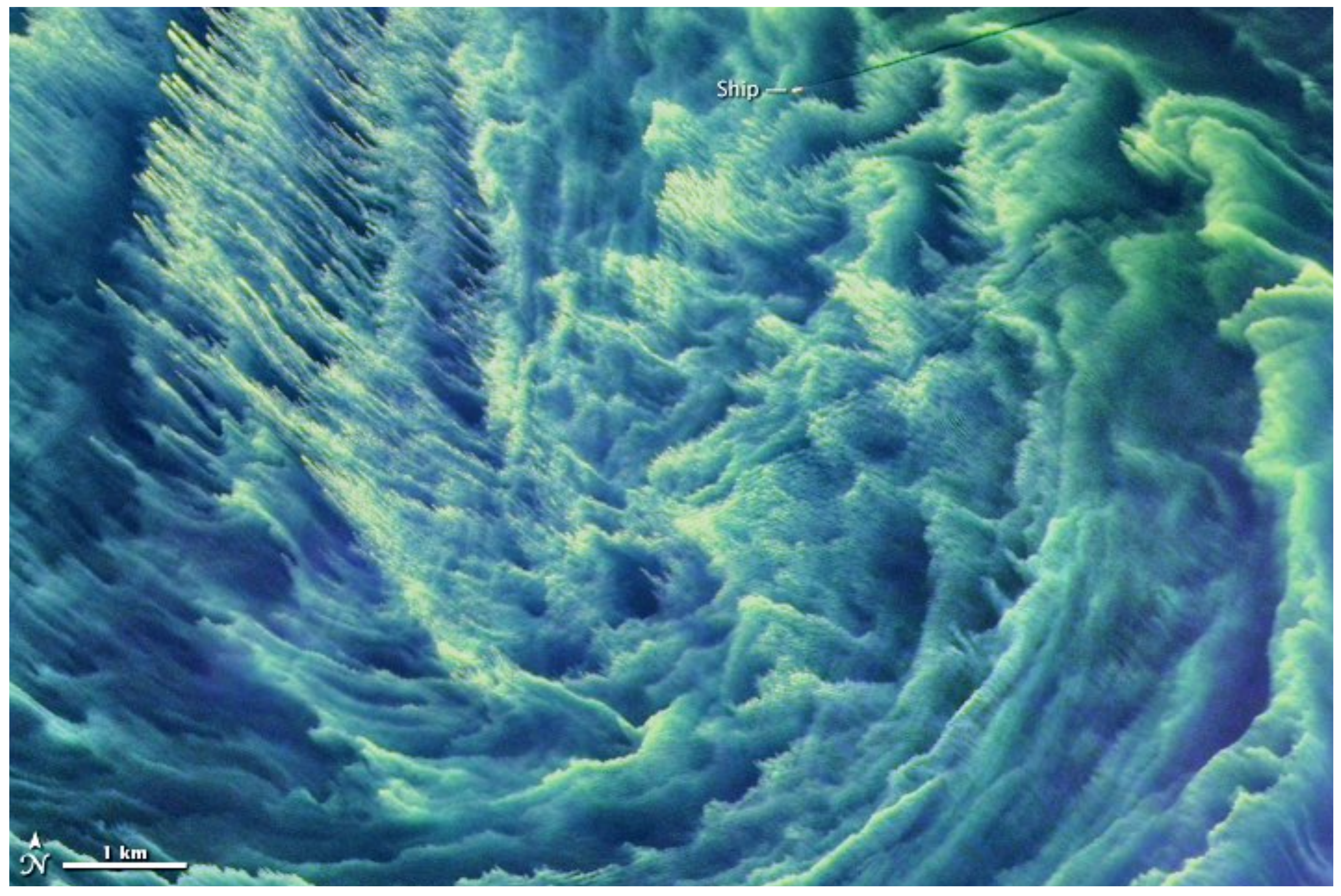
TOWARDS MULTI-SCALE MODELING OF OCEAN SURFACE TURBULENT MIXING USING COUPLED MPAS-OCEAN AND PALM



Bloom of cyanobacteria in the Baltic Sea
https://landsat.visibleearth.nasa.gov/view.php?id=86449

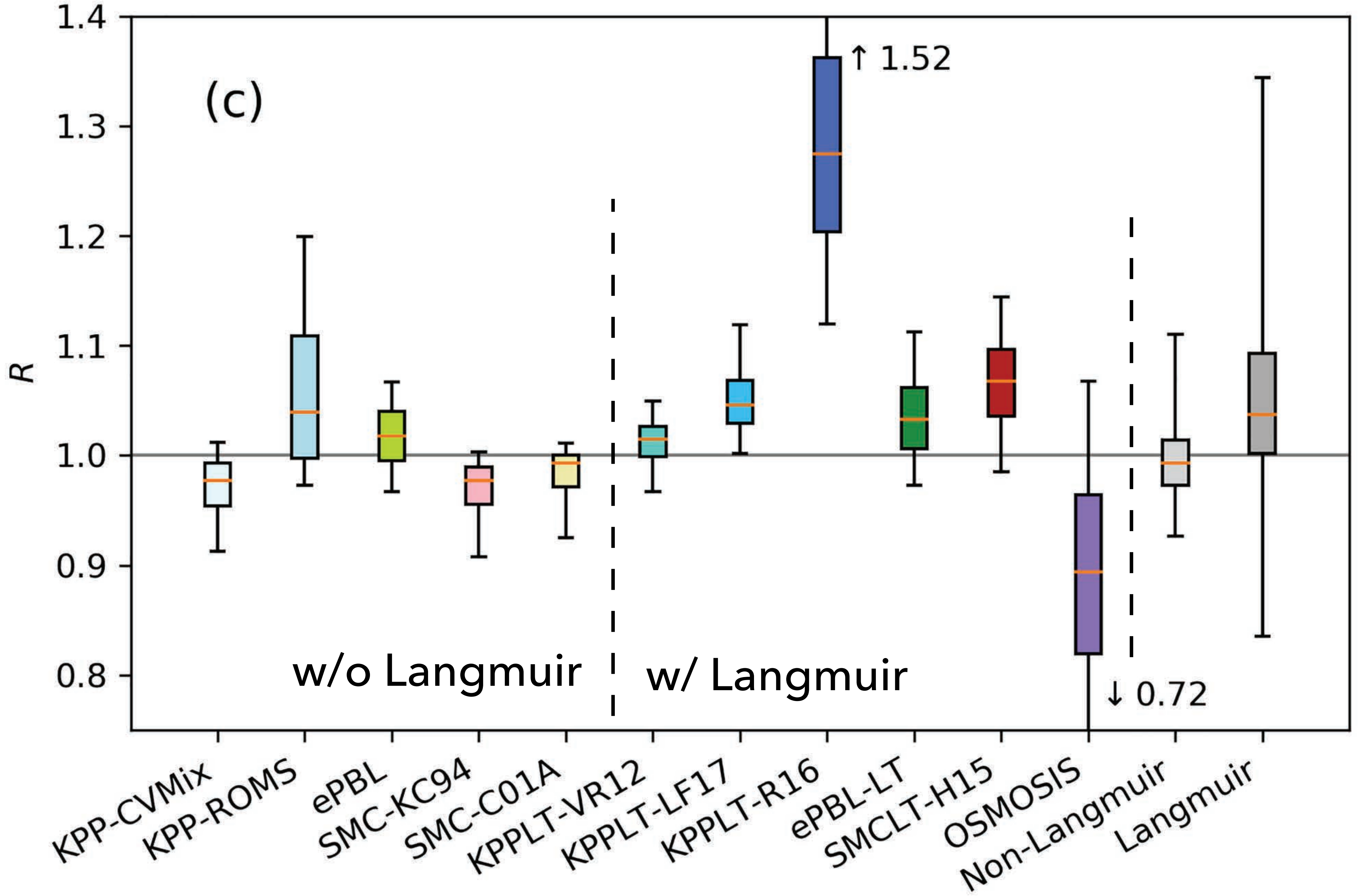
WHY OCEAN TURBULENT MIXING?

- Effects on large scales:
  - Ocean absorbs a great amount of excess heat and CO_2 from the atmosphere (~1/4 of anthropogenic CO_2 and ~90% of total warming in the climate system)
  - Distribution of the absorbed heat and CO_2
  - The capability of the ocean to buffer the climate change
- Effects on small scales:
  - Transport and dispersion of ocean pollutants (e.g., spilled oil, plastic wastes)
  - Availability of nutrients for biogeochemical processes
  - Sediment transport in an estuarine environment

MODELING THE OCEAN TURBULENT MIXING

- Ocean turbulent mixing is parameterized in ocean general circulation models (GCM) / Earth System Models
- Significant discrepancies exist among many ocean turbulent mixing parameterizations
- Large eddy simulations (LES) are important tools in developing / validating ocean turbulent mixing parameterizations, given the scarcity of direct measurements

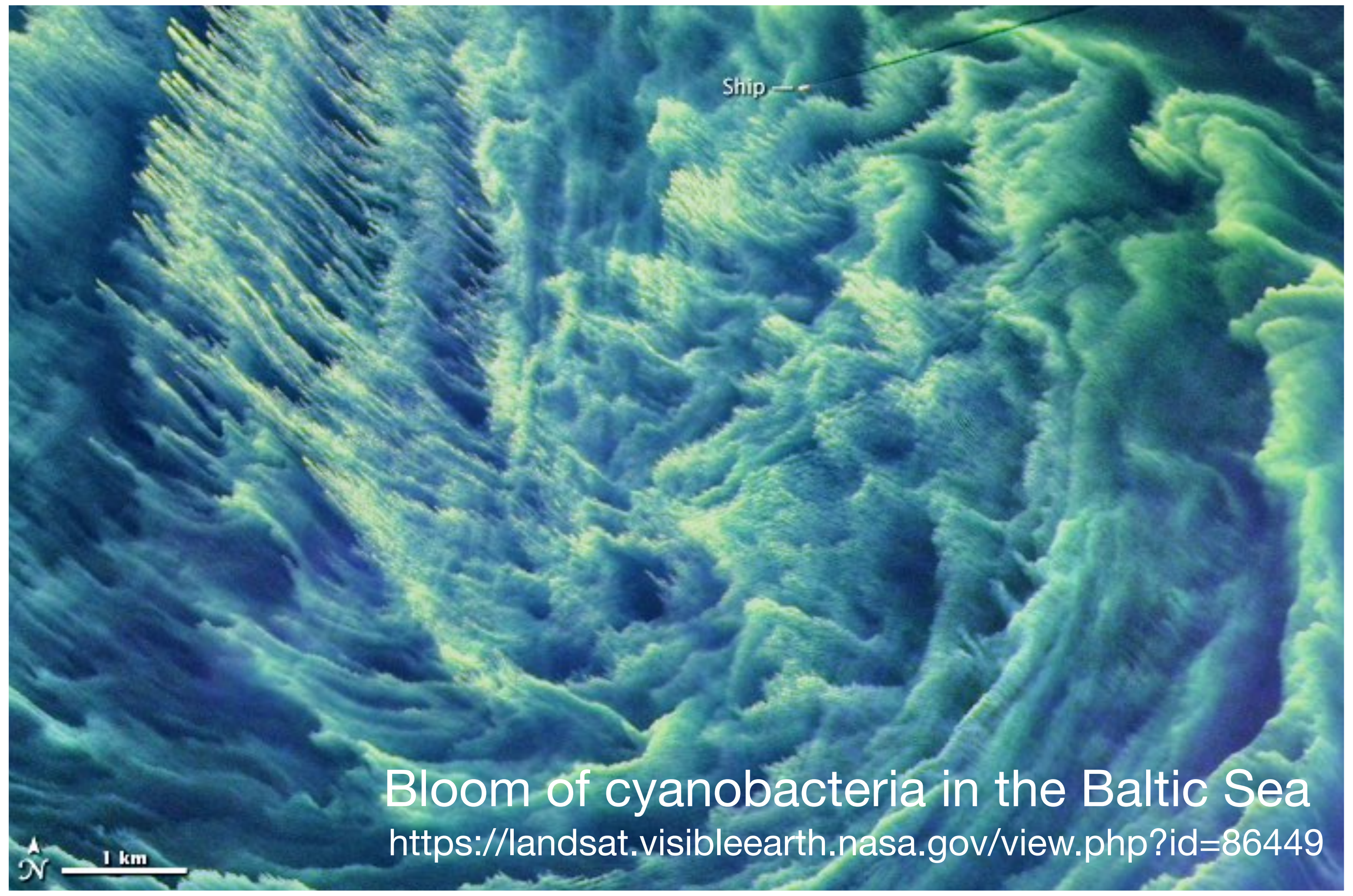
Discrepancies among 11 ocean surface vertical mixing parameterizations



Li et al., 2019, JAMES

WHY MULTI-SCALE MODELING?

- Ocean mixing is multi-scale
  - Boundary layer turbulence [~$\mathcal{O}(1)$ m]
  - Submesoscale eddies & fronts [~$\mathcal{O}(10^3)$ m]
  - Mesoscale eddies [~$\mathcal{O}(10^5)$ m]
- Interactions across scales matters
- Simulations that resolve all important scales are extremely computationally expensive
- Flexibility of mesh resolution in MPAS-Ocean ⇔ Turbulence-resolving LES



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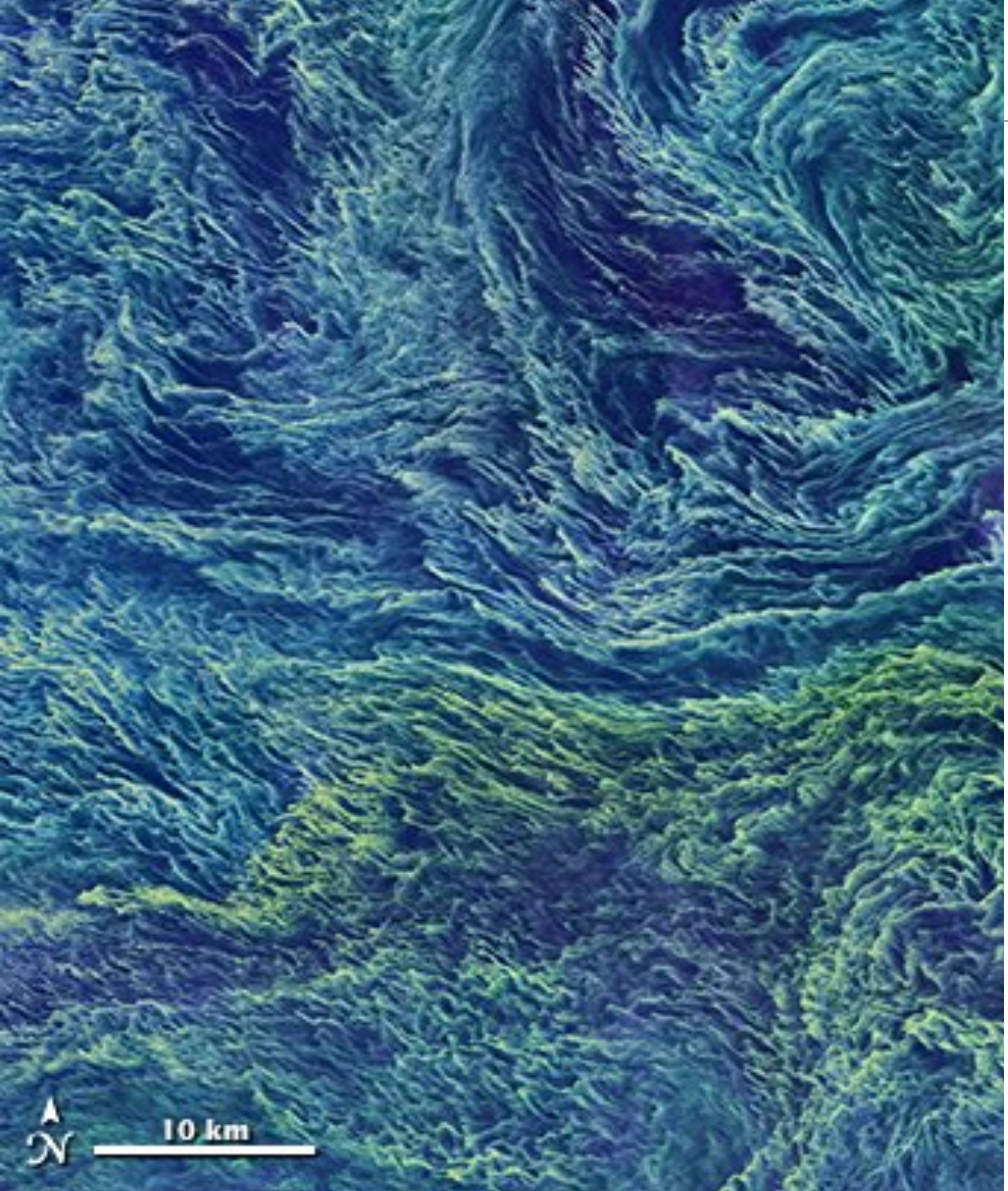
MPAS
Model for Prediction Across Scales

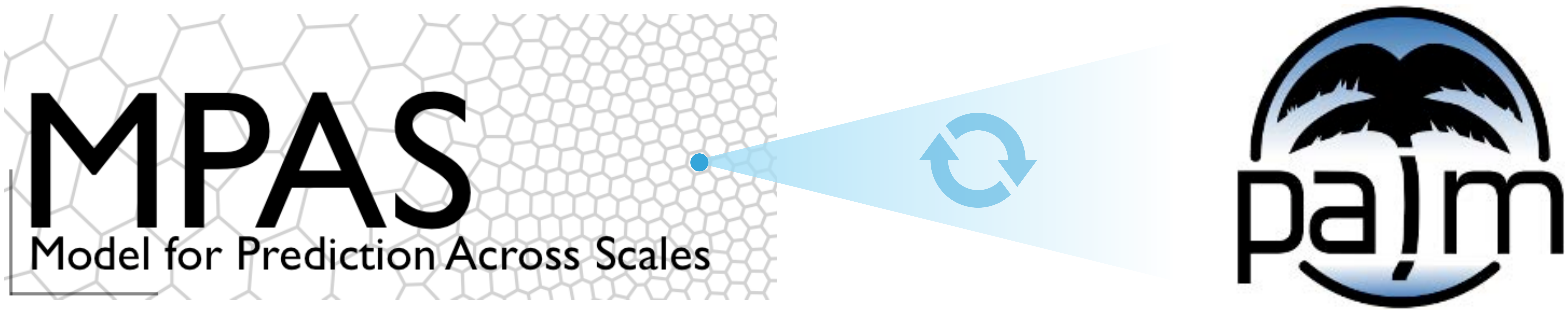


OUTLINE

- Multi-scale modeling
  - Coupling MPAS-Ocean & PALM
  - Porting PALM on GPU
- Evaluation
  - Idealized diurnal cycle
  - Mixed layer eddy
- Moving forward

COUPLING MPAS-OCEAN & PALM

Large-scale **Small-scale**

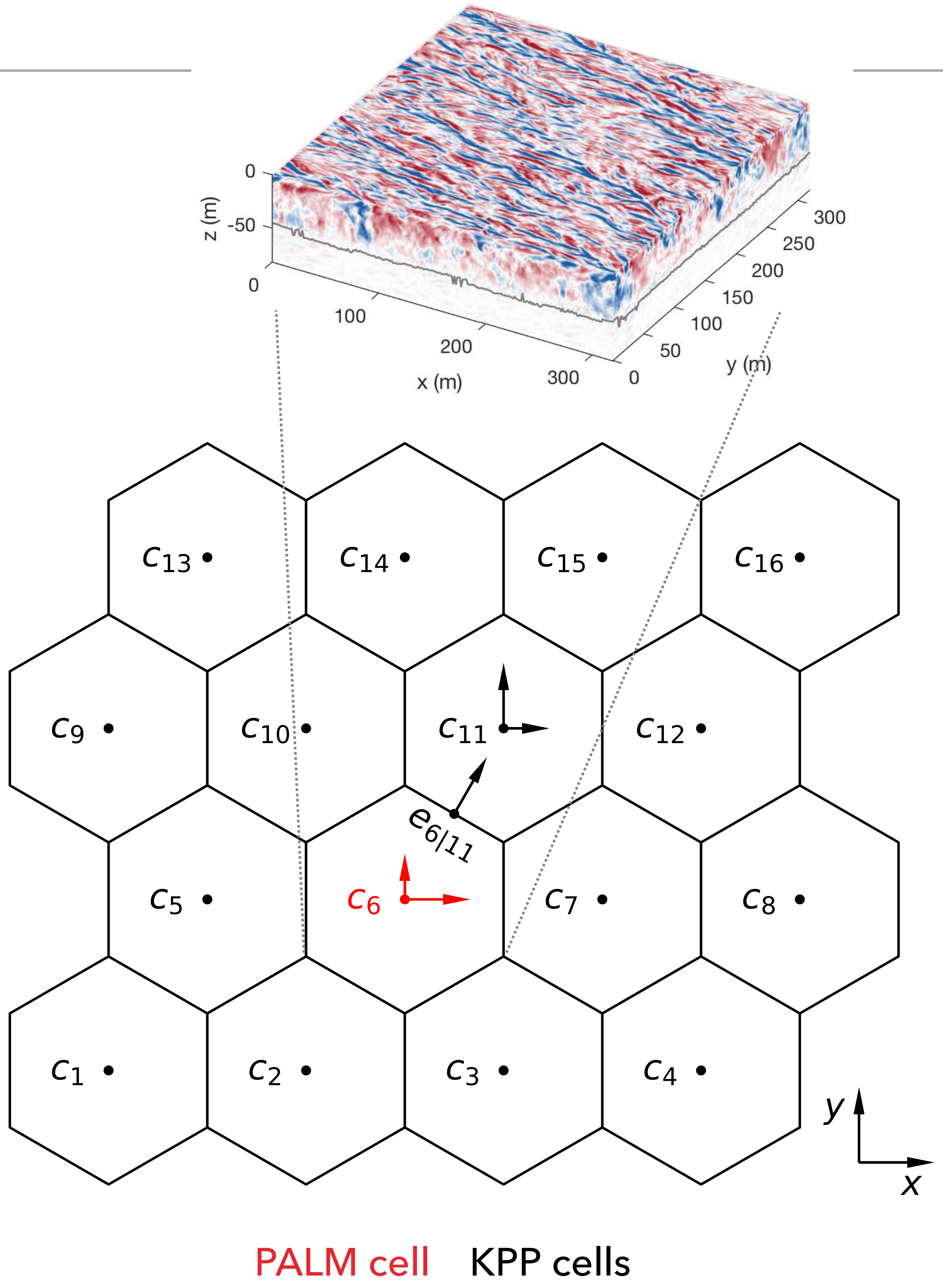


- Ocean general circulation model (GCM)
- Hydrostatic, incompressible, and Boussinesq primitive equations on an unstructured-mesh using finite volume discretization

- Turbulence-resolving large eddy simulation (LES) model
- Non-hydrostatic, incompressible and spatially filtered Navier–Stokes equations with the Boussinesq approximation on Cartesian grid using finite difference discretization

COUPLING MPAS-OCEAN & PALM

- PALM running at the center of some selected grid cells in MPAS-Ocean
- K-profile parameterization (KPP) on other cells
- Coupling
  - Tracers on cell centers
  - Momentum on cell centers vs. on cell edges
- Inconsistency in the momentum?



COUPLING MPAS-OCEAN & PALM

- Consistent large-scale & small-scale

$$\overline{\boldsymbol{u}_h^f} = \boldsymbol{u}_h^c$$
$$\overline{\theta^f} = \theta^c$$

- Small-scale → large-scale

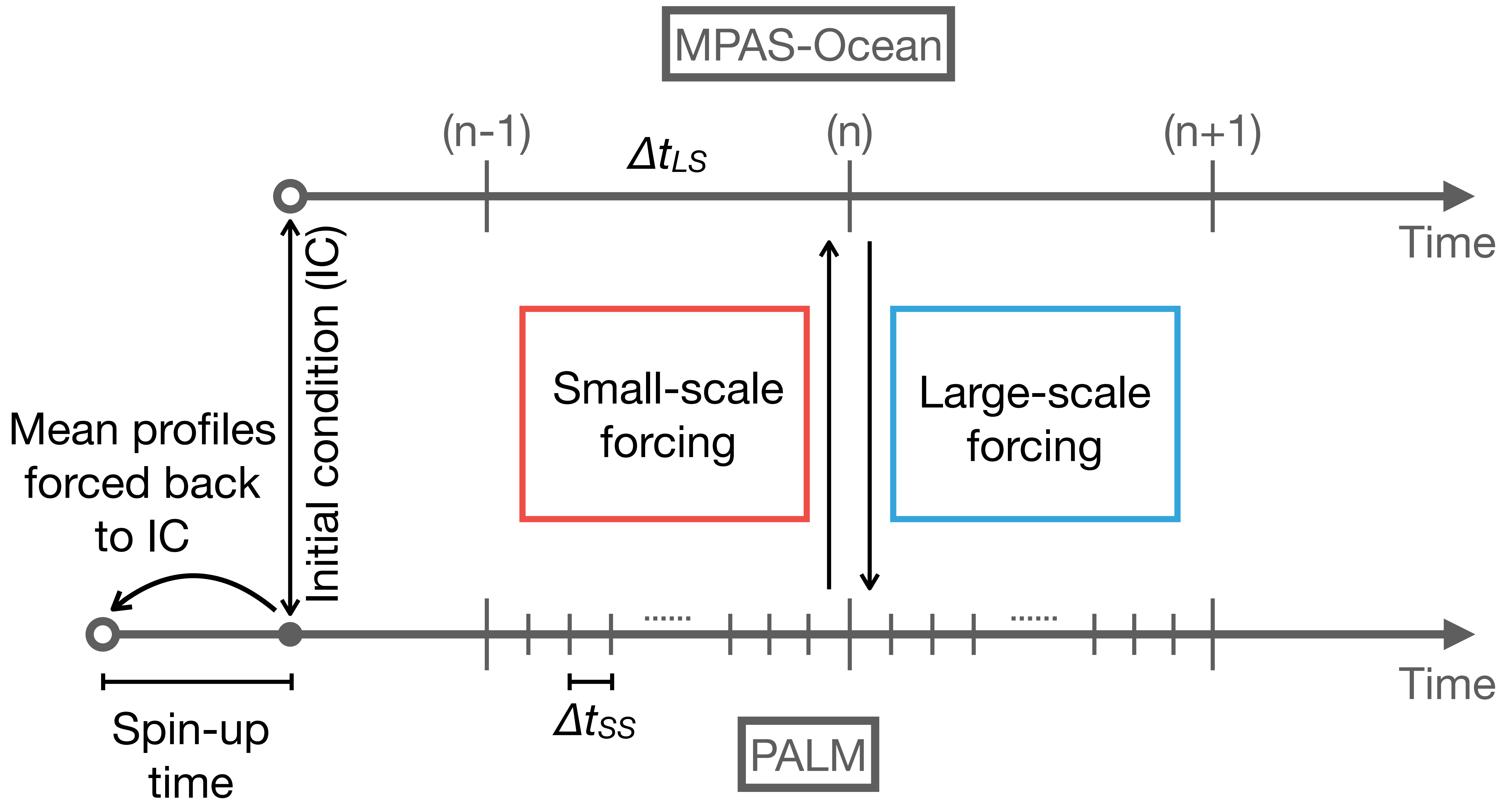
$$\boldsymbol{F}_{\mathrm{SS}}^{\boldsymbol{u}_h} = -\partial_z \overline{w^{f\prime}\boldsymbol{u}_h^{f\prime}}$$
$$F_{\mathrm{SS}}^{\theta} = -\partial_z \overline{w^{f\prime}\theta^{f\prime}}$$

- Large-scale → small-scale

$$\boldsymbol{F}_{\mathrm{LS}}^{\boldsymbol{u}} = \frac{\boldsymbol{u}_h^c - \overline{\boldsymbol{u}_h^f}}{\tau_{\mathrm{LS}}^{\boldsymbol{u}}}$$
$$F_{\mathrm{LS}}^{\theta} = \frac{\theta^c - \overline{\theta^f}}{\tau_{\mathrm{LS}}^{\theta}}$$

Momentum: $\partial_t \boldsymbol{u}^c = \cdots + \boldsymbol{F}_{\mathrm{SS}}^{\boldsymbol{u}_h}$

Tracers: $\partial_t \theta^c = \cdots + F_{\mathrm{SS}}^{\theta}$



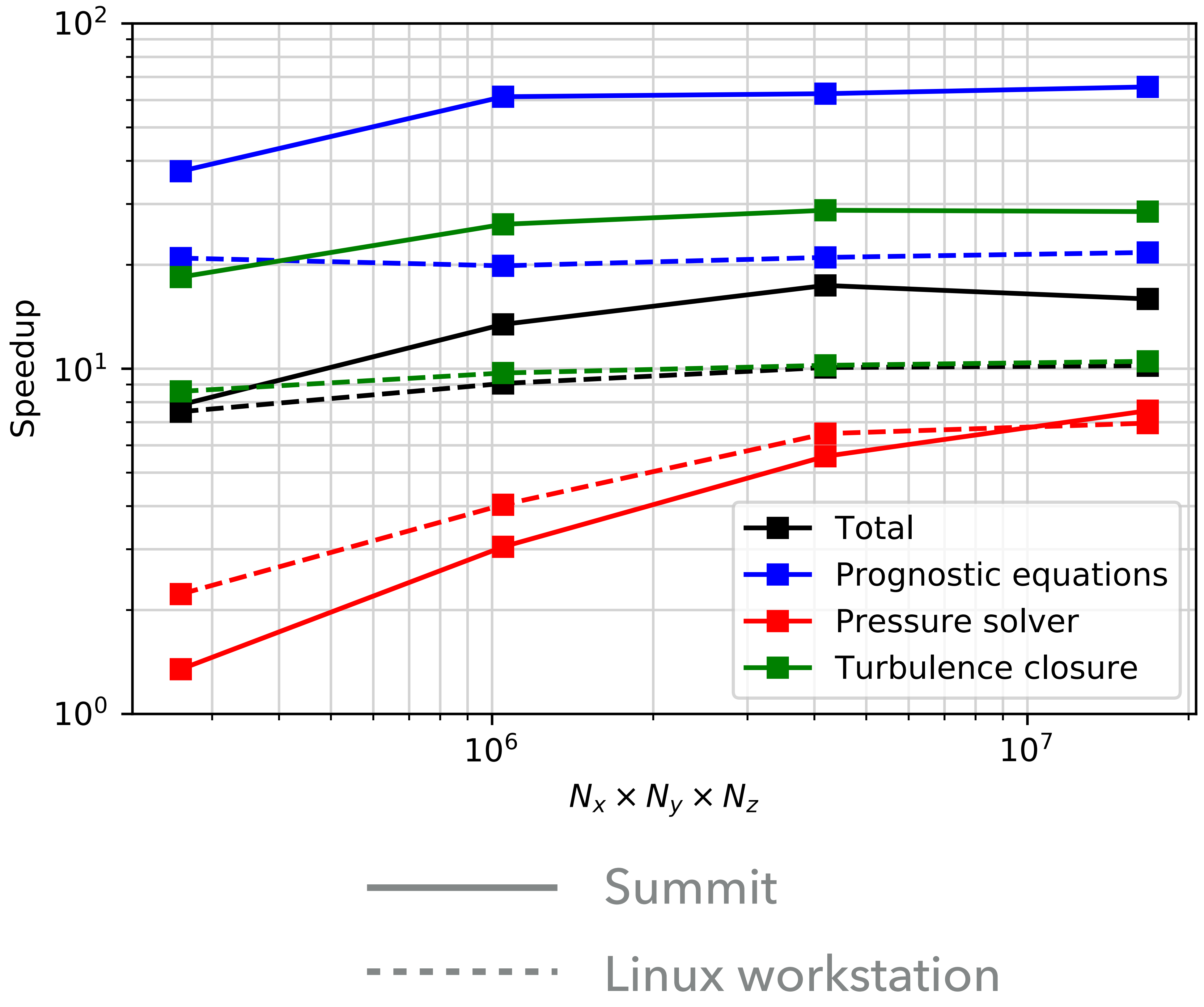
Momentum: $\partial_t \boldsymbol{u}^f = \cdots + \boldsymbol{F}_{\mathrm{LS}}^{\boldsymbol{u}_h}$

Tracers: $\partial_t \theta^f = \cdots + F_{\mathrm{LS}}^{\theta}$

PORTING PALM ON GPU

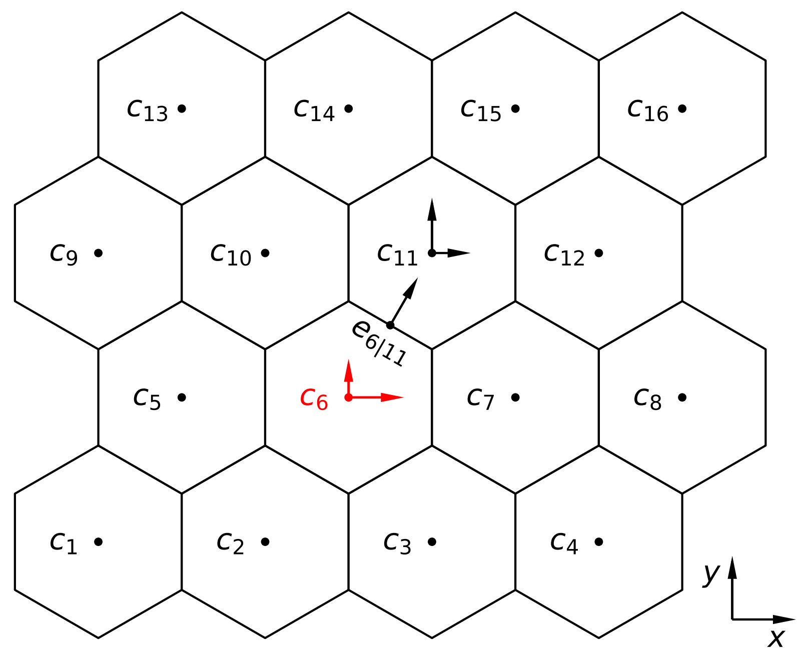
- Running PALM in MPAS-Ocean is computationally expensive
- PALM is ported on GPU using OpenACC and CUDA Fast Fourier Transform library (cuFFT)
- Benchmark
  - Linux workstation (Intel Xeon Silver 4112 @ 2.60GHz + NVIDIA Quadro RTX 4000)
  - Summit
  - Speedup factor = runtime with 1 CPU / runtime with 1 CPU + 1 GPU (all with 1 MPI task)
  - 10-16 times overall speedup

Speedup factor vs. mesh size

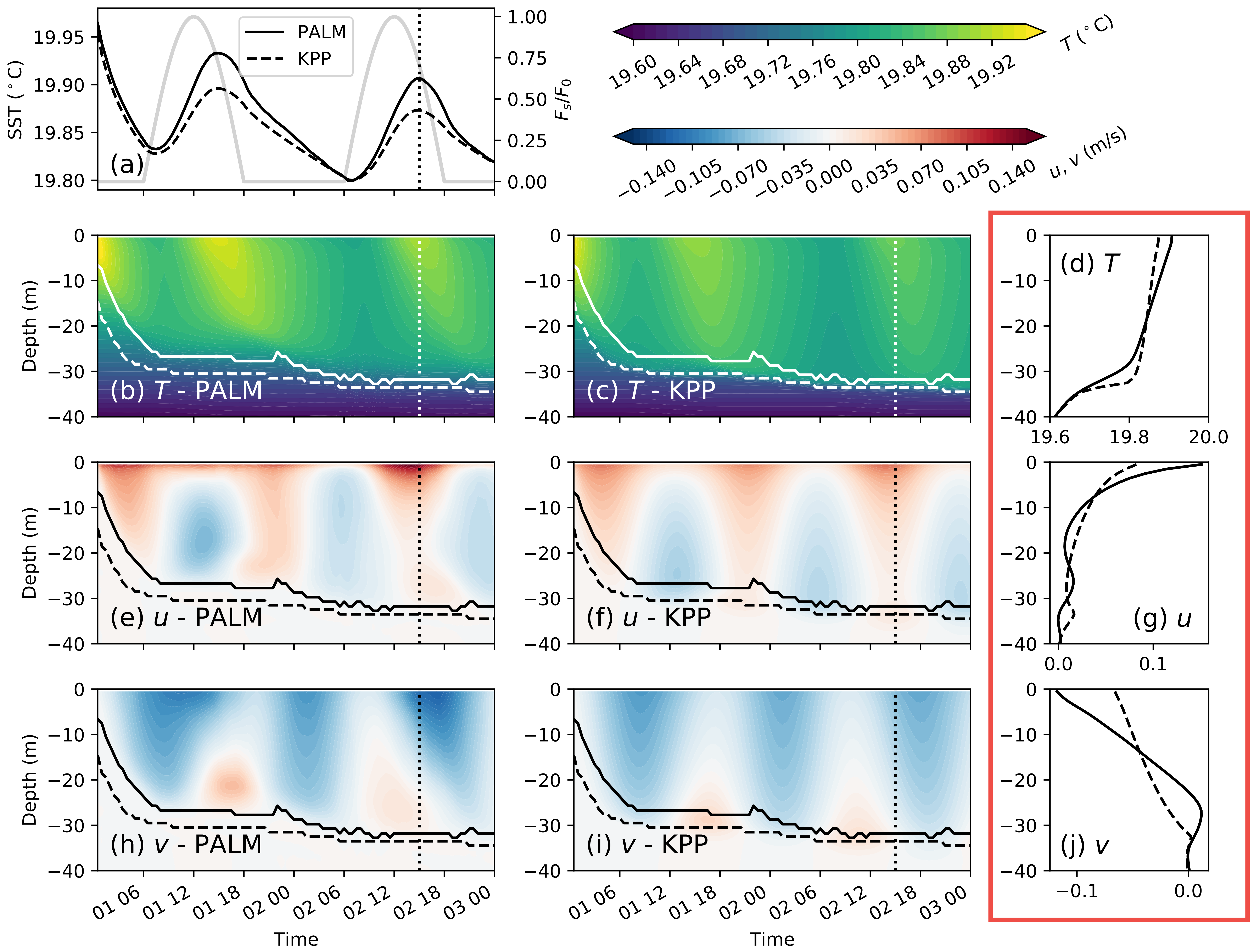


IDEALIZED DIURNAL CYCLE

- Setup:
  - 16 columns in a “single column” mode
  - Idealized diurnal diurnal heating + constant cooling
  - Constant wind stress
  - Rotation ($f = 1.028 \times 10^{-4}$ s-1)



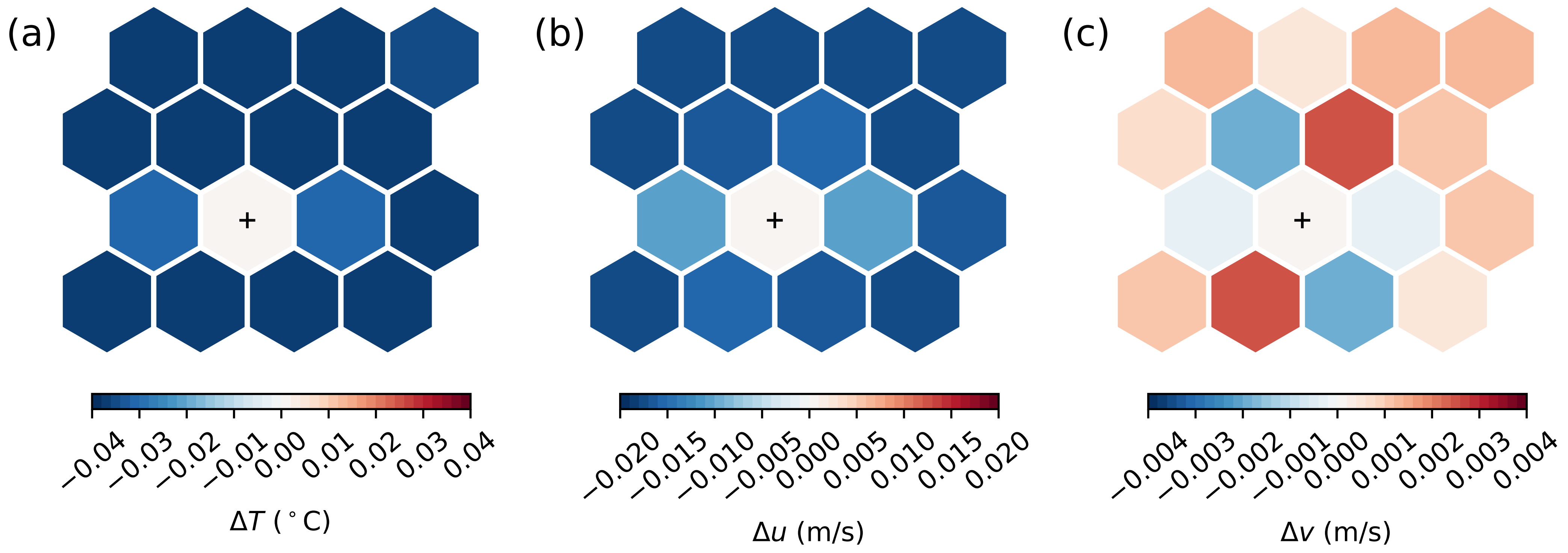
Standalone PALM and KPP



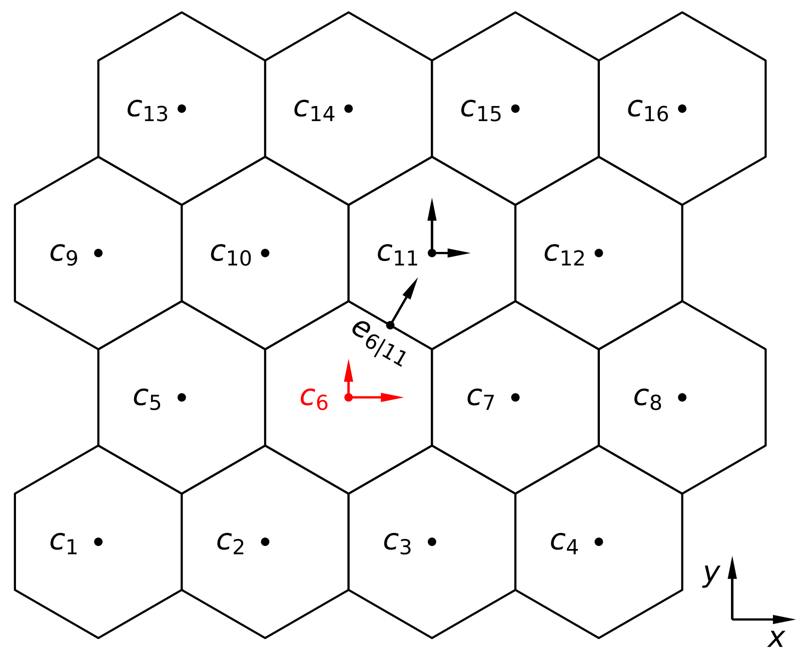
IDEALIZED DIURNAL CYCLE

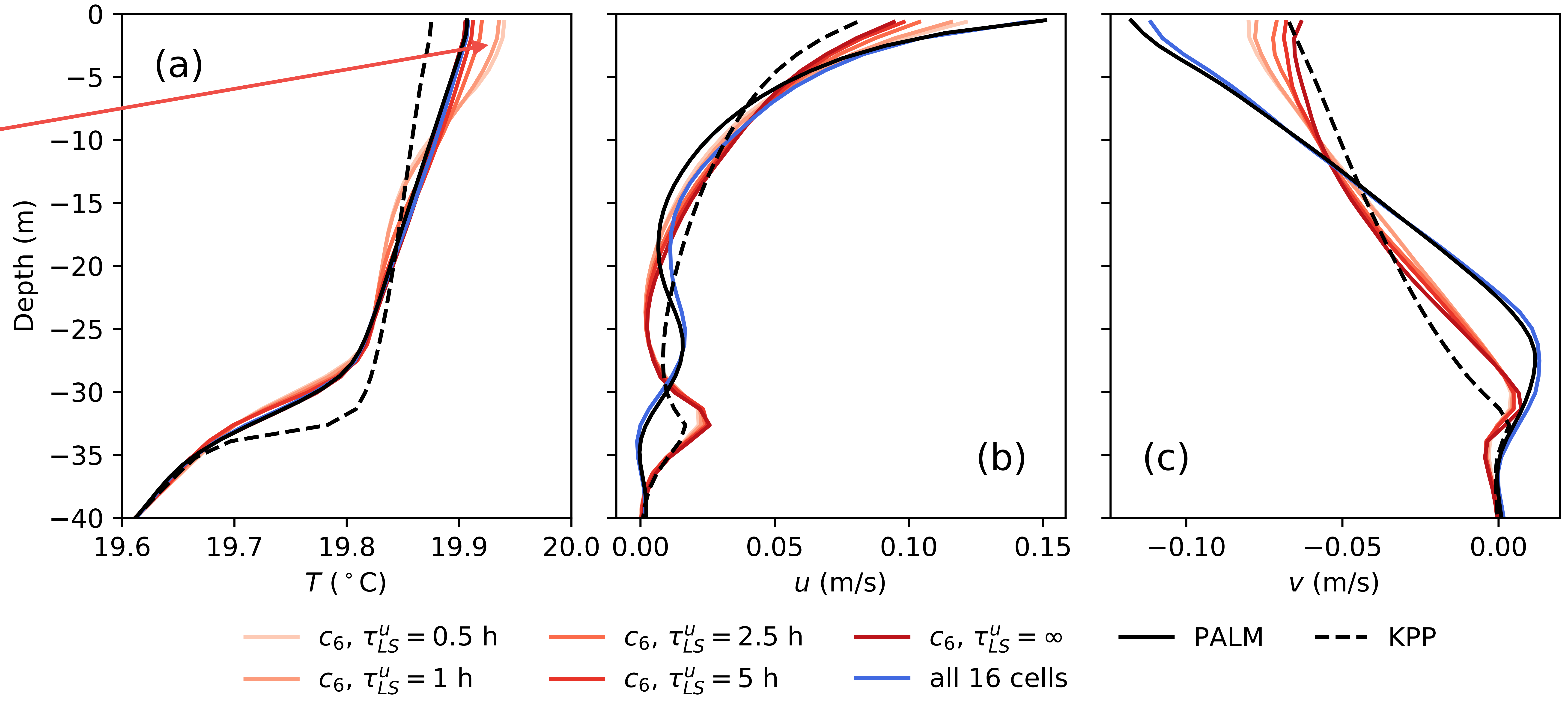
- Sensitivity to the relaxation time scale for the momentum

Surface temperature and velocity differences



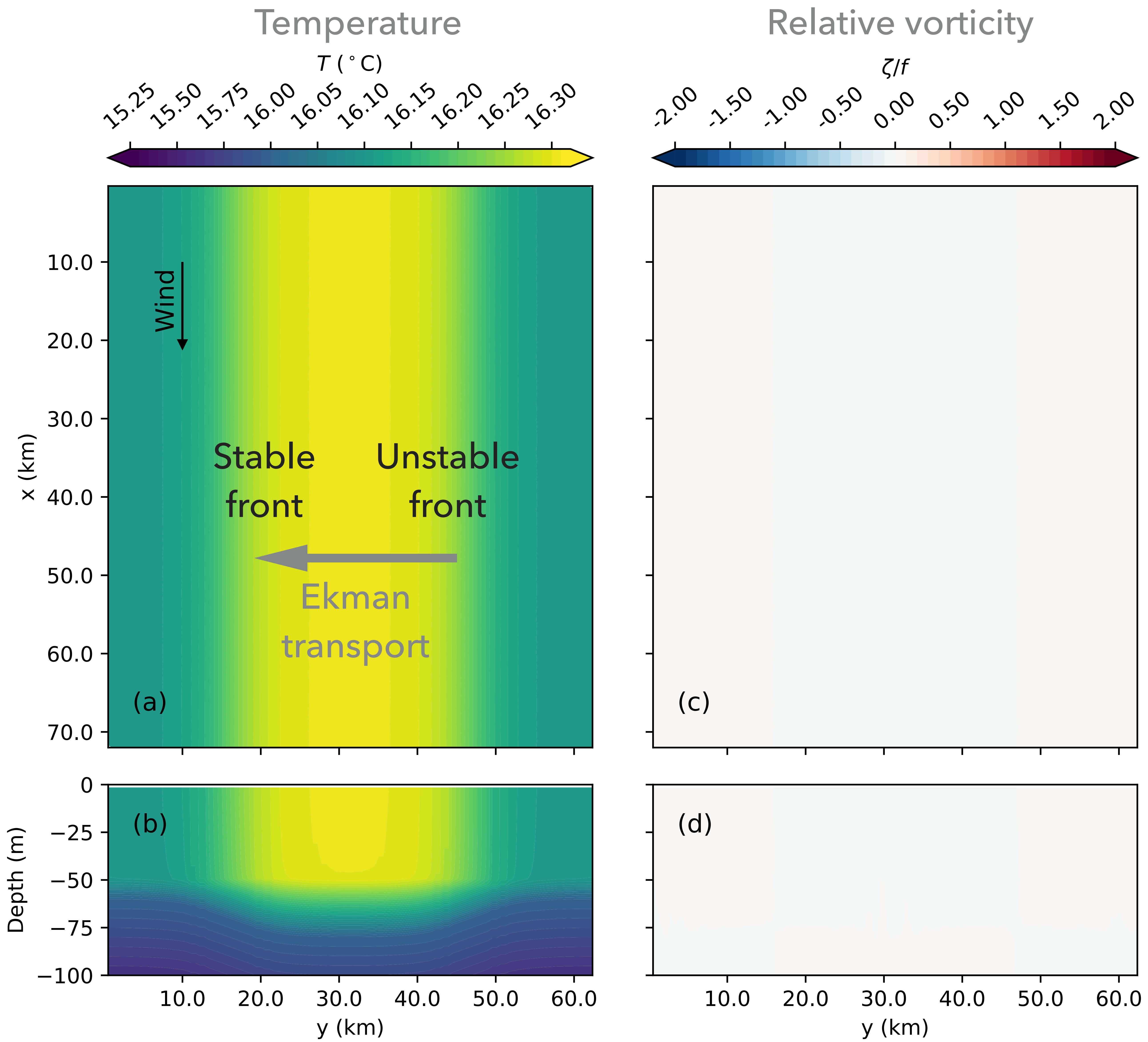
A surface warm layer develops when the momentum is tightly coupled – influence of the neighboring KPP cells





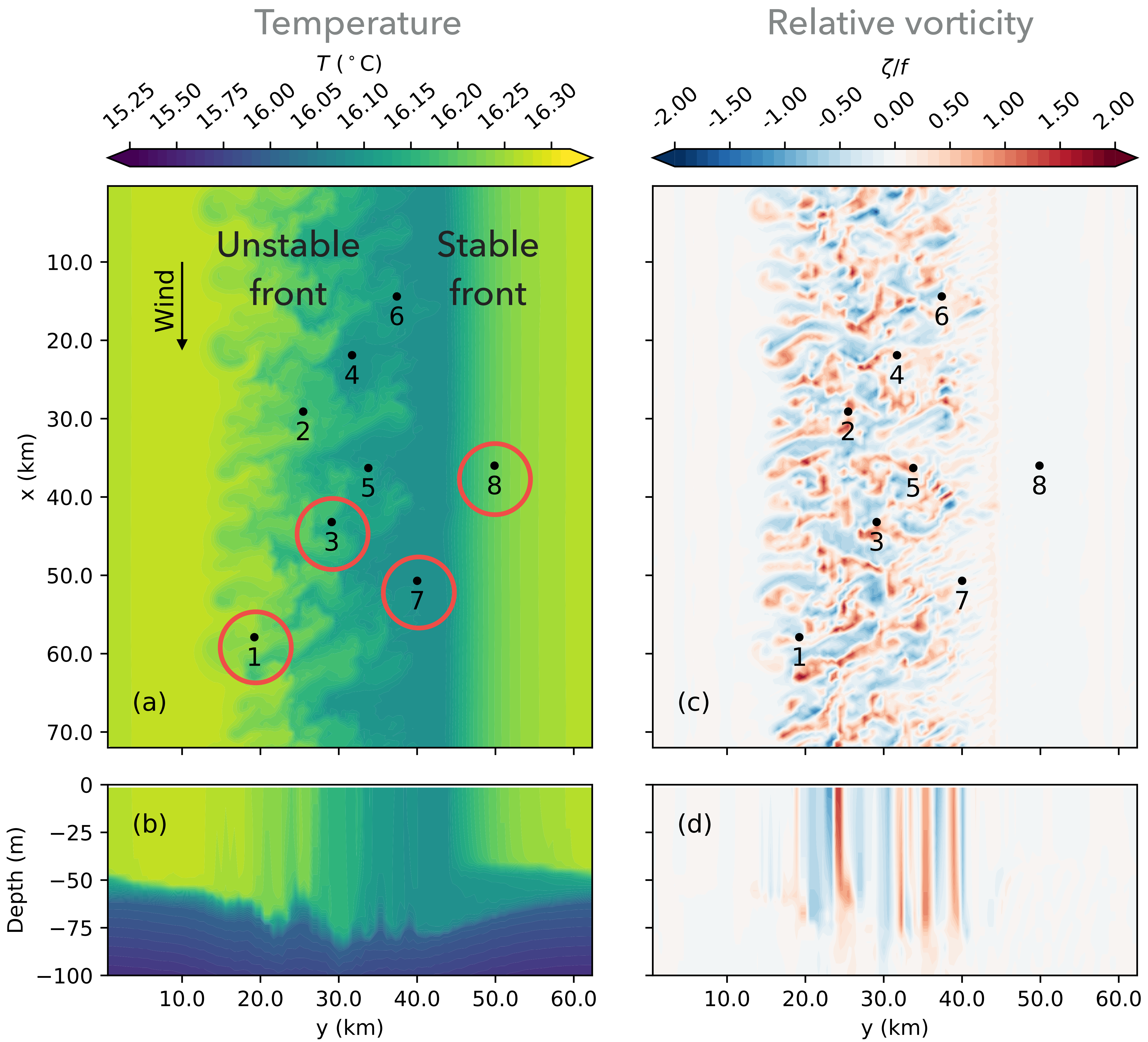
MIXED LAYER EDDY

- Turbulent mixing in the presence of large-scale forcing due to mixed layer eddies
- Setup:
  - Warm filament, zero initial velocity (unbalanced)
  - Doubly periodic domain (72 km $\times$ 62.4 km with 14400 cells / $\Delta l = 600$ m)
  - No surface heat flux
  - Constant wind stress
  - Rotation ($f = 1 \times 10^{-4}$ s-1)



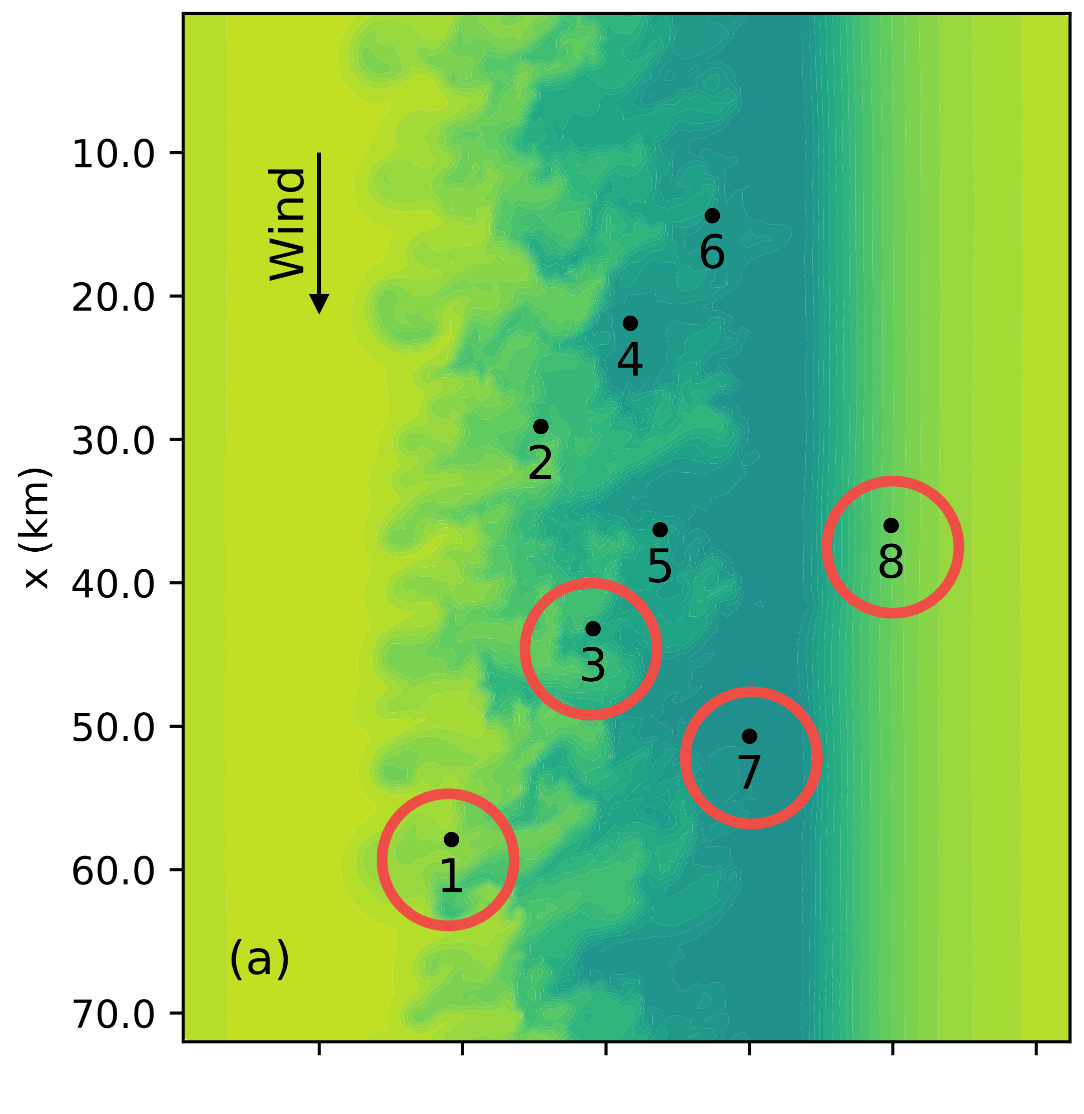
MIXED LAYER EDDY

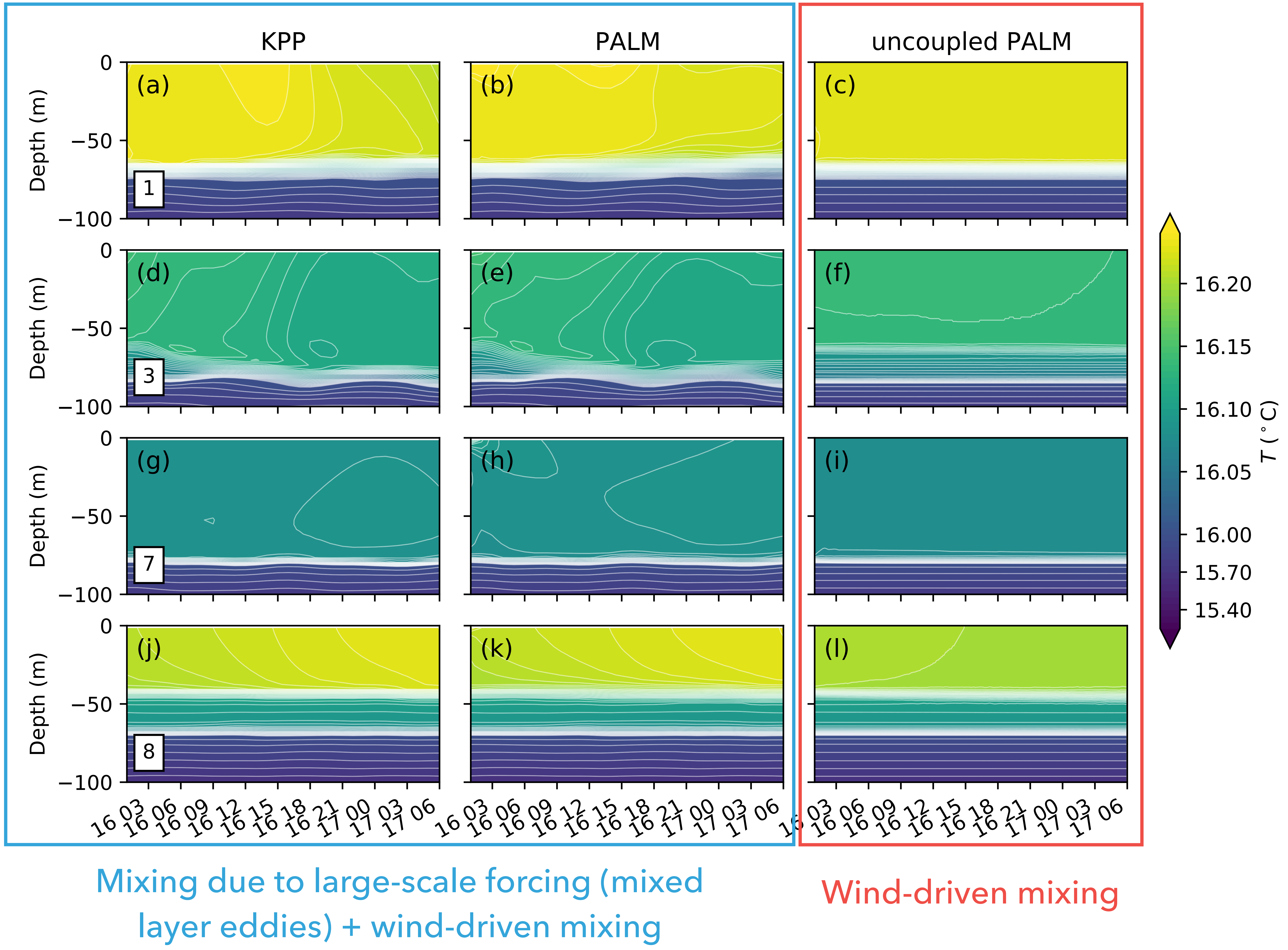
- Spin up with KPP for 15 days
- 30-hour simulations with 3 configurations:
  - Continue with KPP
  - PALM running on 8 grid cells with two-way coupling
  - PALM running on 8 grid cells with no coupling

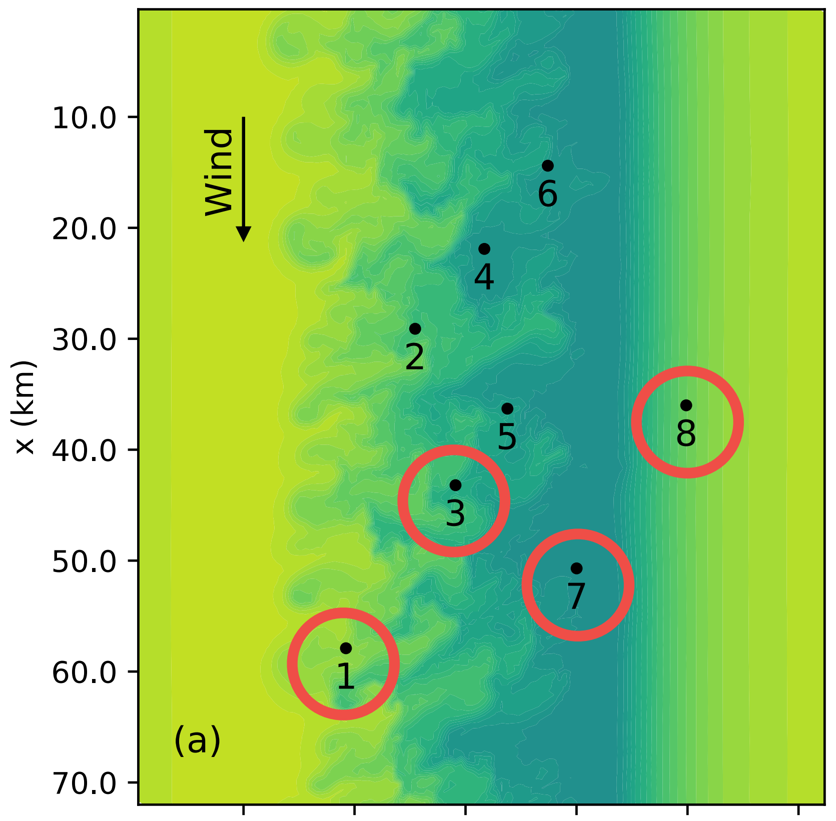


MIXED LAYER EDDY

- Time evolution of temperature profiles at four locations

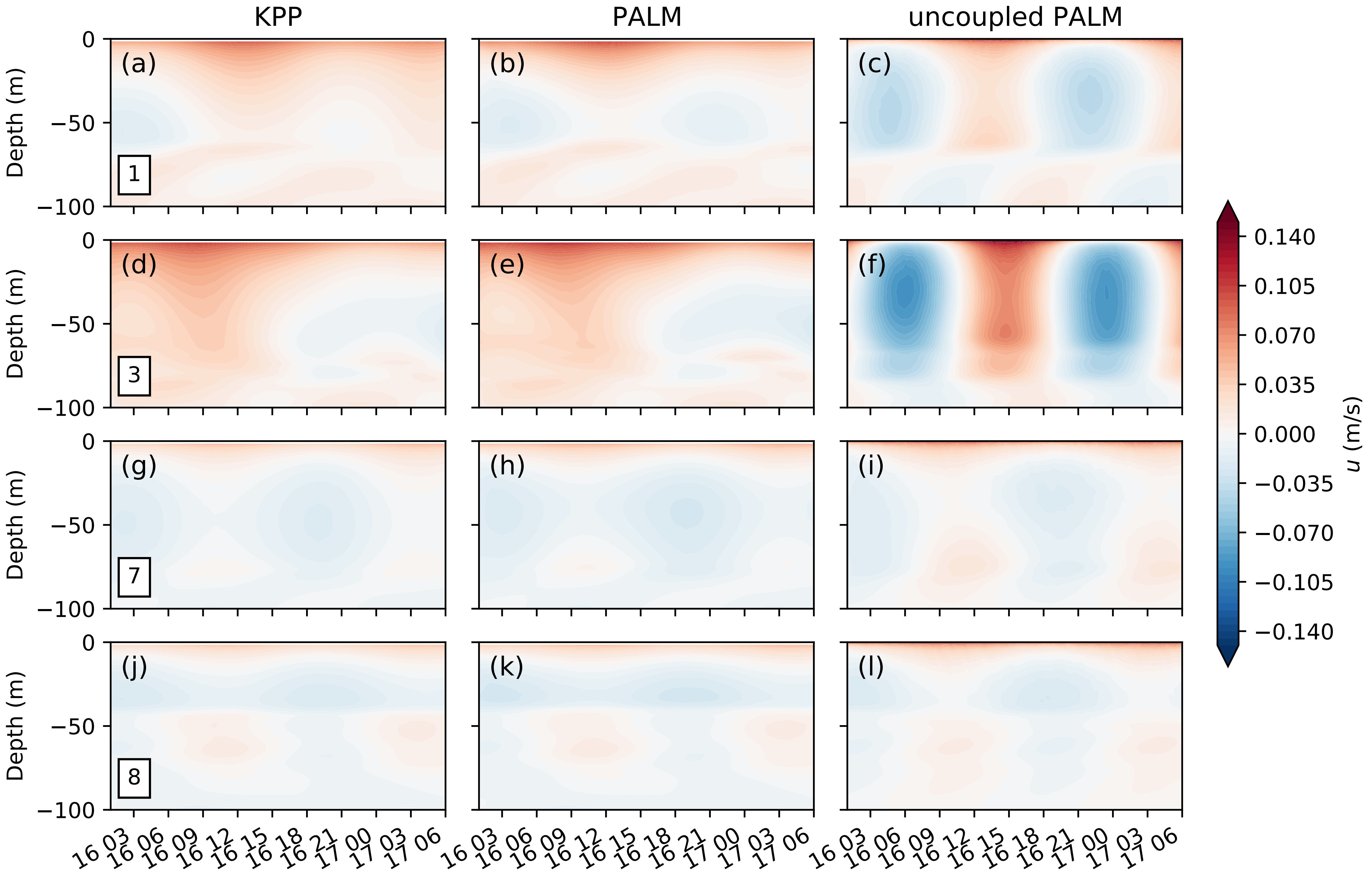




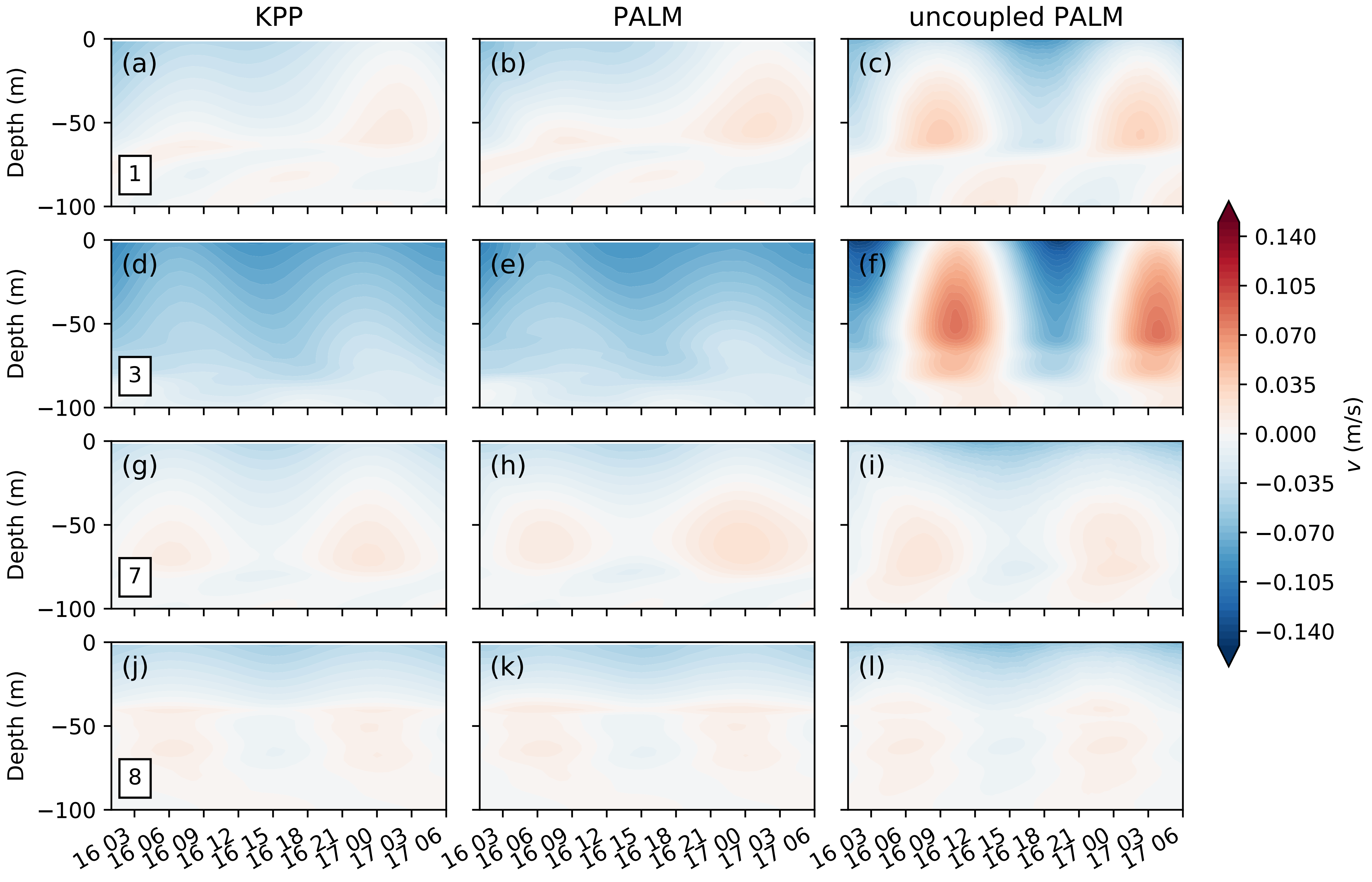


MIXED LAYER EDDY

- Time evolution of velocity profiles at four locations



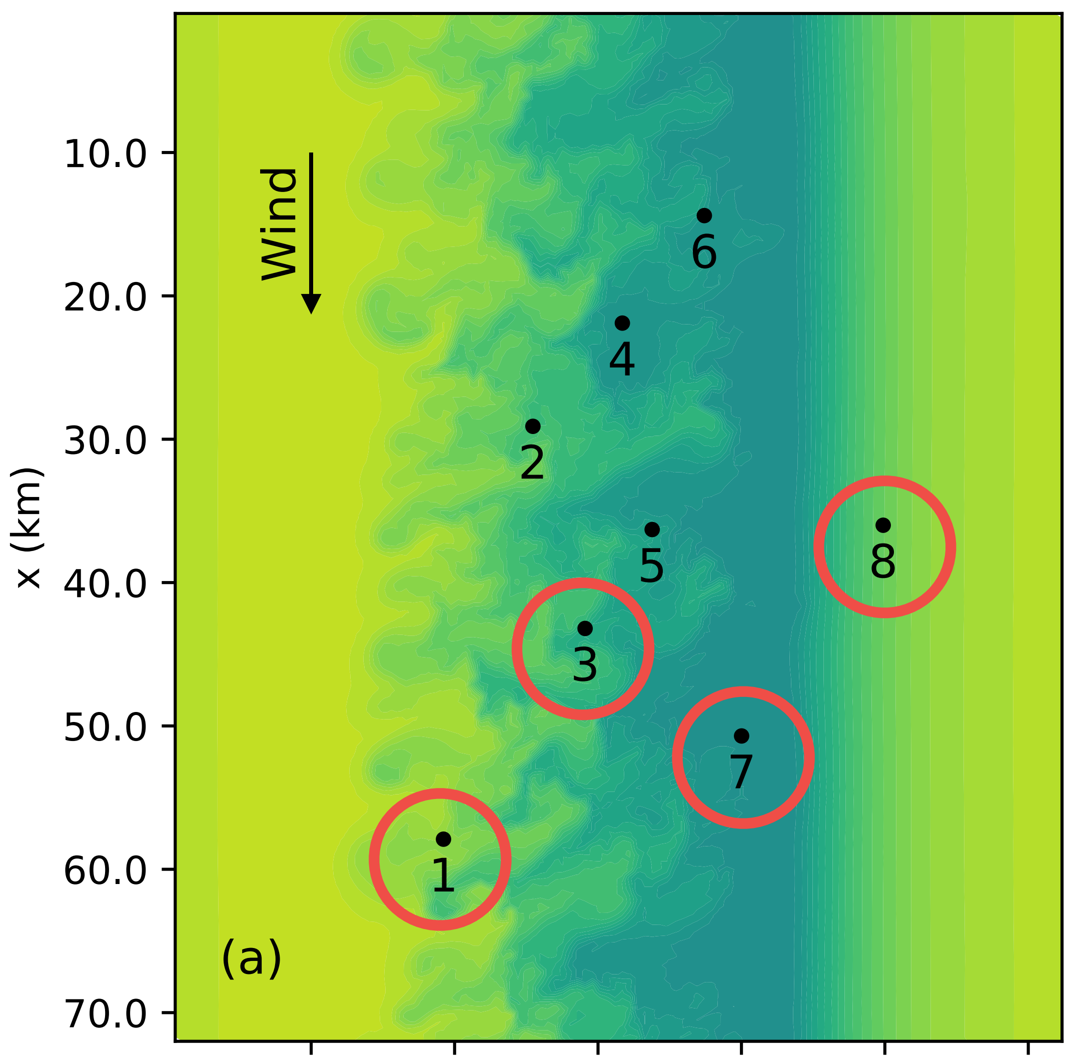
u (m/s)

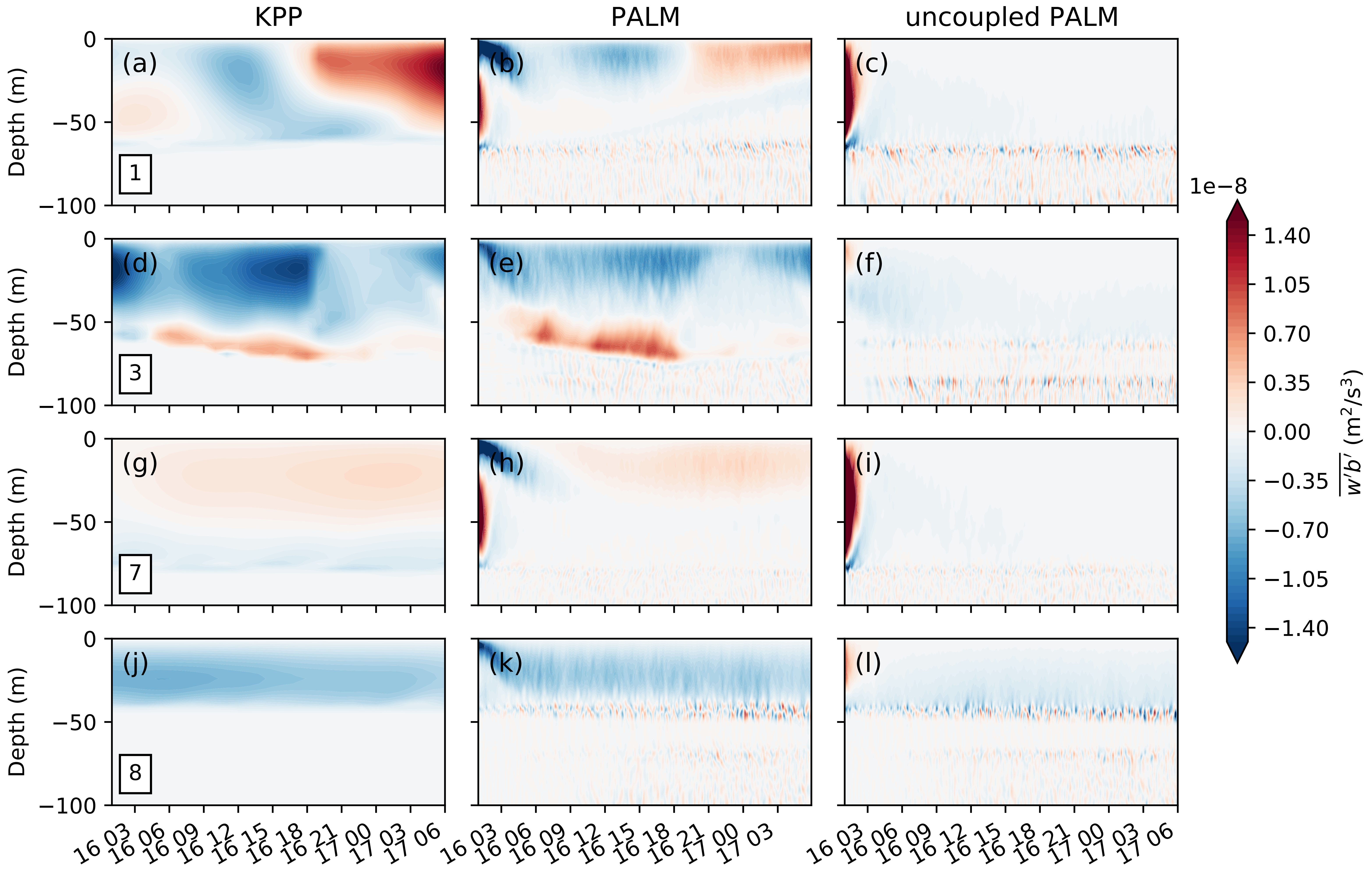


v (m/s)

MIXED LAYER EDDY

- Time evolution of buoyancy flux profiles at four locations





SUMMARY

- Building towards a multi-scale modeling framework to study the ocean surface turbulent mixing, and their interactions with larger-scale processes
- Flexible coupling strategy between MPAS-Ocean and PALM
- PALM is ported on GPU → over x10 speedup
- Simple test cases
  - To evaluate the functionality of the coupling framework
  - To expose potential issues for future work

MOVING FORWARD

- Lateral gradients in the coupling – allowing, e.g., baroclinic instability in the small-scale dynamics

$$\boldsymbol{F}^{\boldsymbol{u}}_{\mathrm{LS}} = \cdots - \boldsymbol{u}^{f\prime}_{h} \cdot \nabla^{c}_{h}\boldsymbol{u}^{c}$$
$$F^{\theta}_{\mathrm{LS}} = \cdots - \boldsymbol{u}^{f\prime}_{h} \cdot \nabla^{c}_{h}\theta^{c}$$

- Focused process study of ocean turbulent mixing in the presence of large-scale processes
  - PALM running on the finest grid cells of MPAS-Ocean in focused regions
- Parameter space exploration: LES of ocean turbulent mixing under various forcing conditions with and without large-scale forcing, e.g., under hurricane conditions
- Exploring the possibility of improving the simulation results of a GCM by having high-fidelity representations of the turbulent mixing at only a few locations

REFERENCES

- Li, Q., & Van Roekel, L. Towards multiscale modeling of ocean surface turbulent mixing using coupled MPAS-Ocean v6.3 and PALM v5.0. Geoscientific Model Development. In Review. https://doi.org/10.5194/gmd-2020-262

THANK YOU!