ATMOSPHERIC BOUNDARY LAYER SIMULATION AND SUBGRID-SCALE DYNAMICS

1. An Introduction to Outdoor LES

2. Observations and SGS Model Equations

3. LES Applications

FUTURE PETASCALE COMPUTING

What's petascale computing?

- Next generation of massively parallel supercomputers
- Petaflop $\Longrightarrow$ 1,000 trillion operations per second
- Employ $\mathcal{O}(10^5 - 10^6)$ processors!
- Cost $\sim$ \$200 M, power consumption 10-20 MW
- One of the first peta-machines will be "Blue Waters" in 2011 see http://www.ncsa.uiuc.edu/BlueWaters/
- Sustained performance of 1-2 petaflops

CAN WE MAKE AN LES/DNS OF THE PBL EXECUTE ON A LARGE NUMBER OF PROCESSORS?

LES EQUATIONS FOR DRY ATMOSPHERIC PBL

Momentum

$$\frac{D\overline{\mathbf{u}}}{Dt} = -\,\mathbf{f}\times\overline{\mathbf{u}} - \nabla\pi + \hat{\mathbf{z}}g\frac{\overline{\theta}}{\theta_*} - \nabla\cdot\mathbf{T}$$

Scalar

$$\frac{D\overline{b}}{Dt} = -\nabla\cdot\mathbf{B}$$

TKE

$$\frac{De}{Dt} = -\mathbf{T}:\mathbf{S} + \mathbf{B}\cdot\hat{\mathbf{z}} - \mathcal{E} + \nabla\cdot(2\nu_t\nabla e)$$

Subgrid-scale momentum and scalar fluxes

$$\mathbf{T} = \overline{u_i\,u_j} - \overline{u_i}\,\overline{u_j}$$
$$\mathbf{B} = \overline{u_i\,b} - \overline{u_i}\,\overline{b}$$

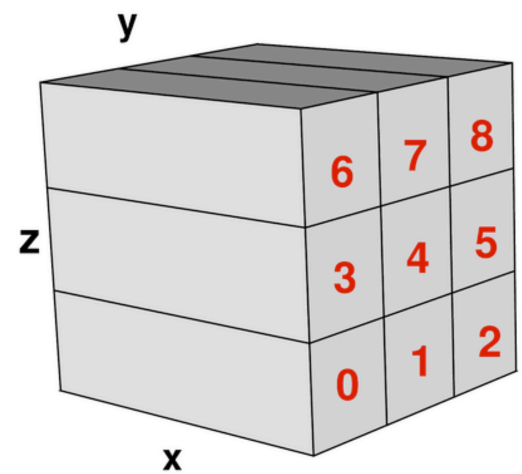
Incompressible Boussinesq flow

$$\nabla\cdot\overline{\mathbf{u}} = 0 \implies \nabla^2\pi = s$$

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

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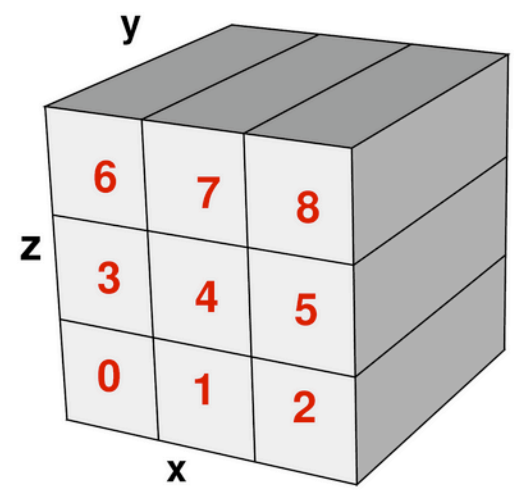

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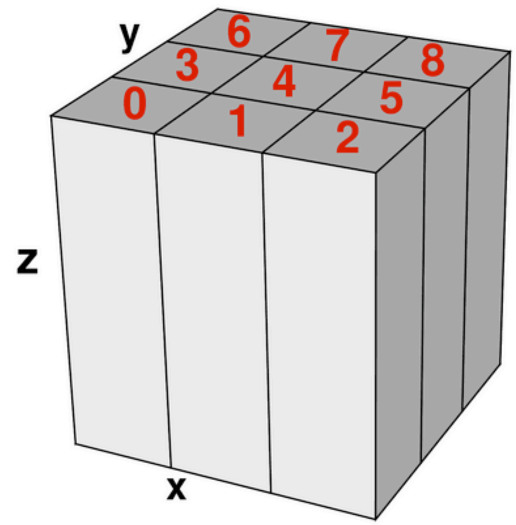

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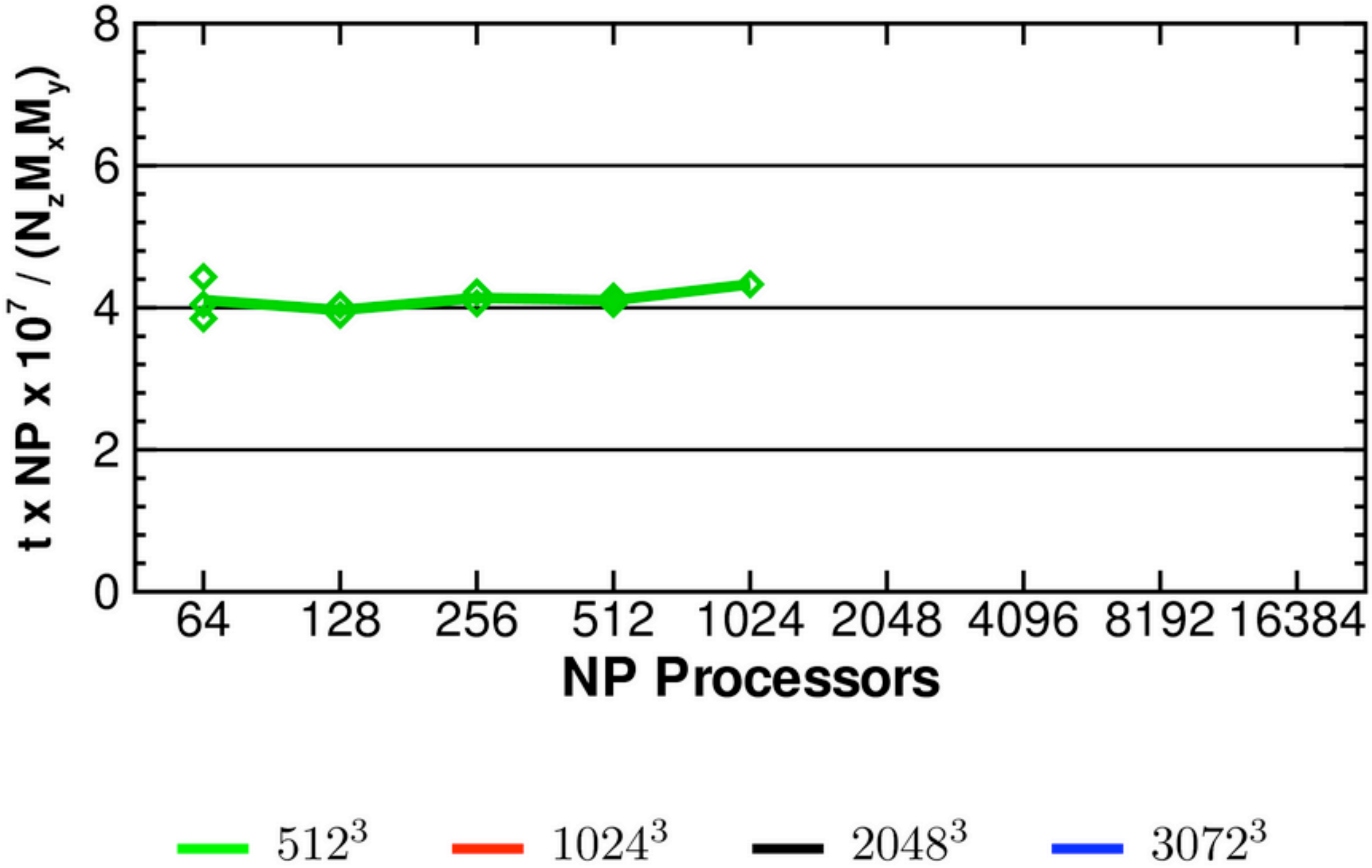
SCALING OF PARALLEL PSEUDOSPECTRAL ALGORITHM WITH 2-D DOMAIN DECOMPOSITION

Cray XT4, NERSC



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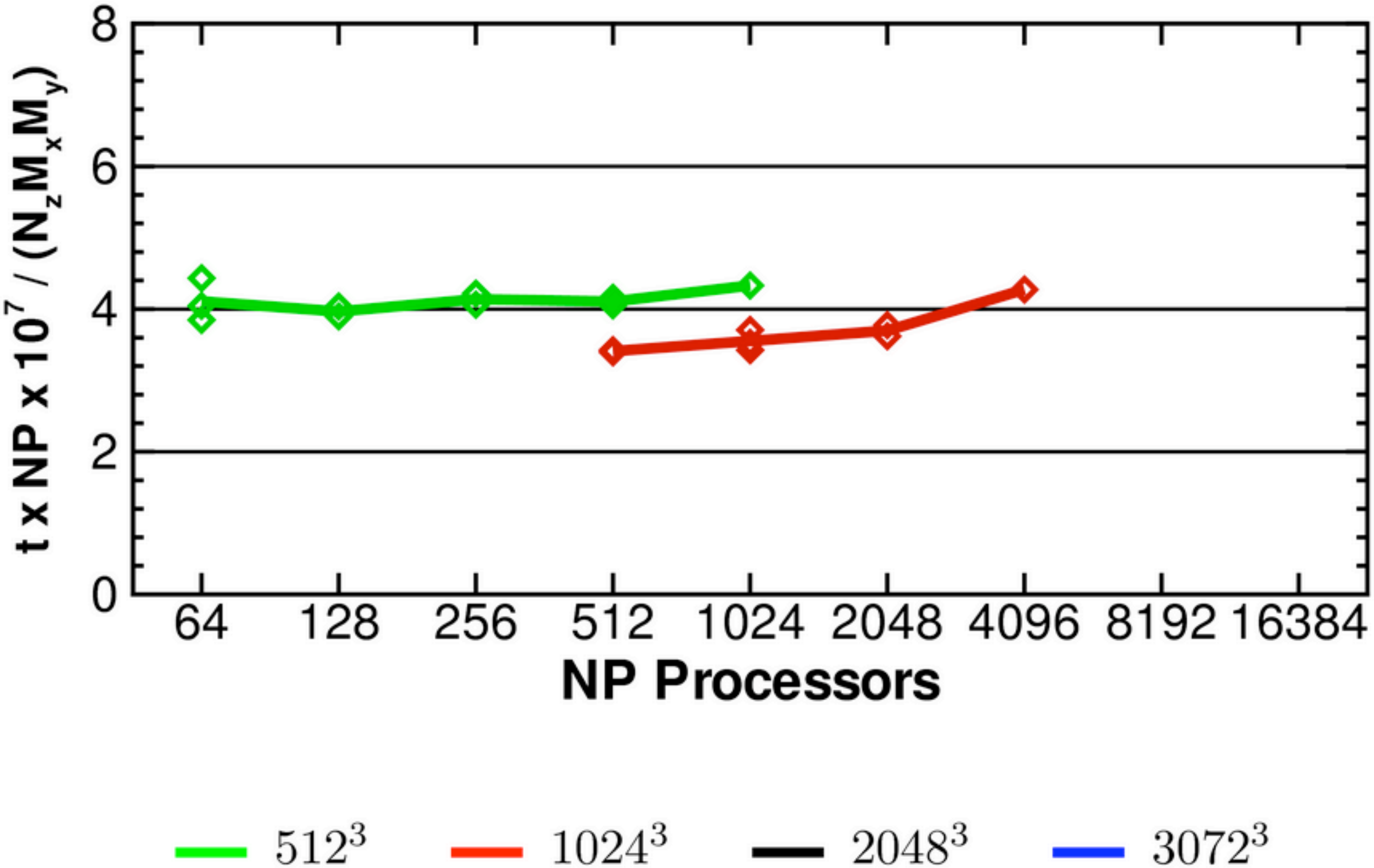

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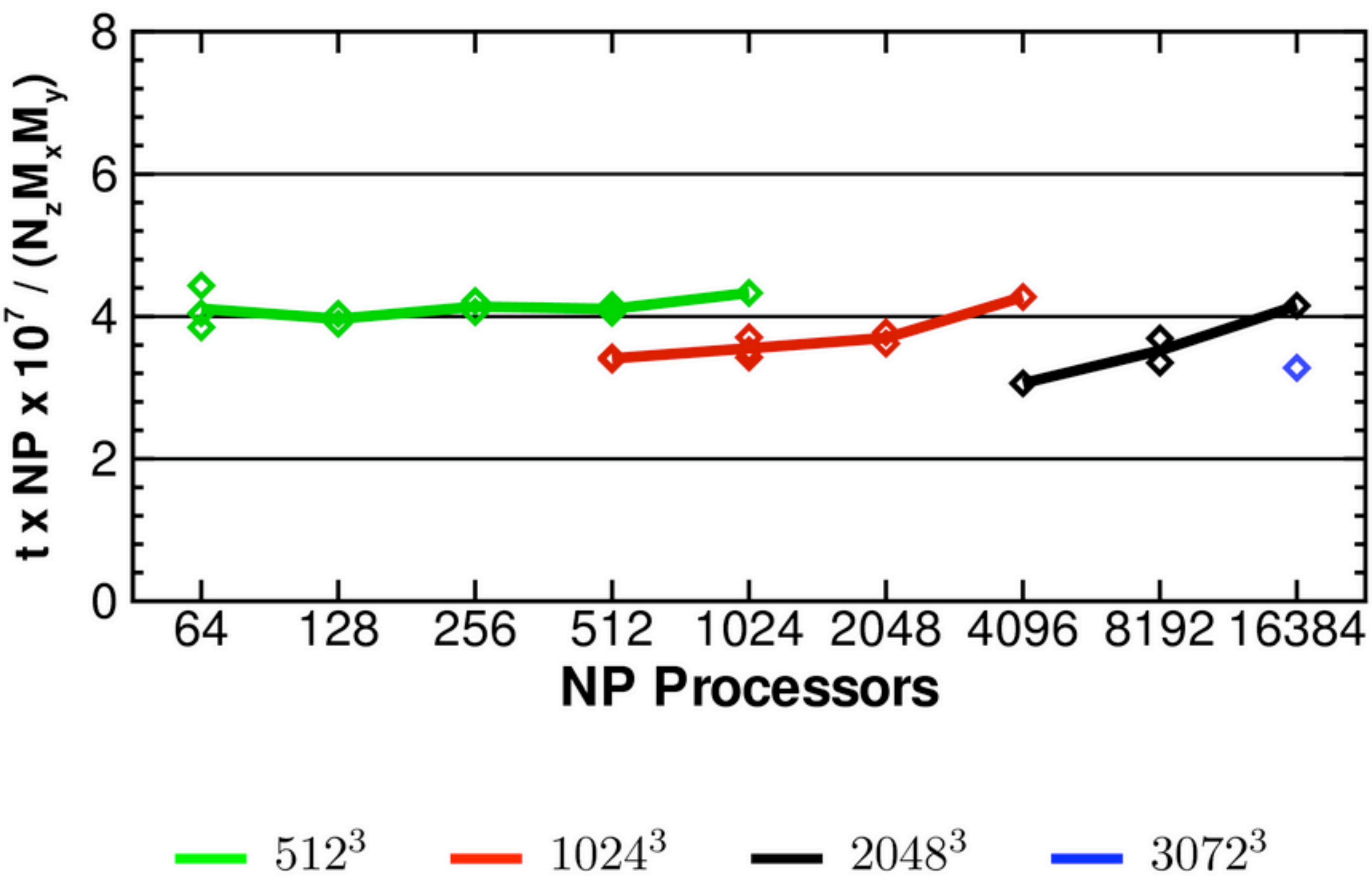
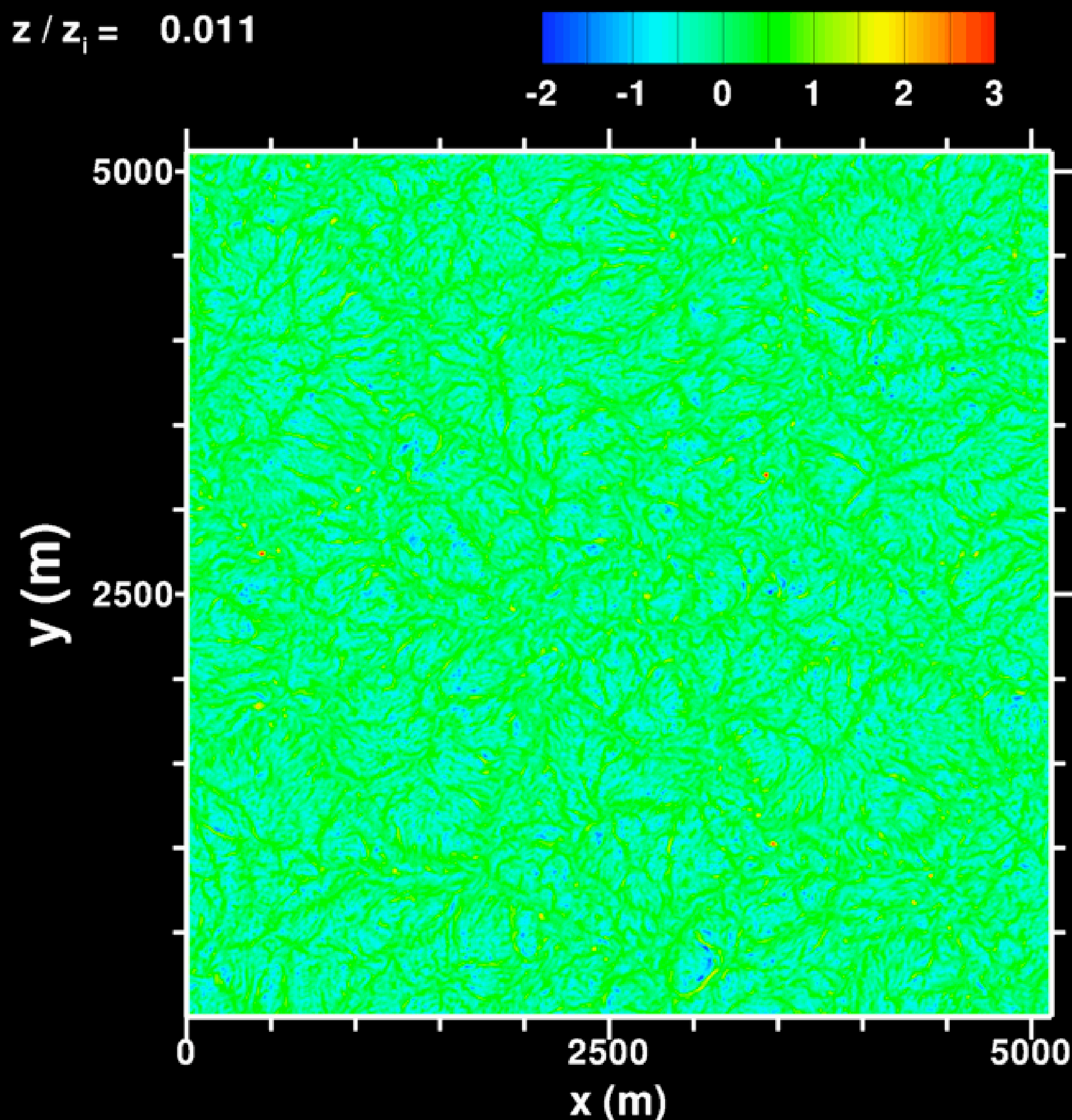


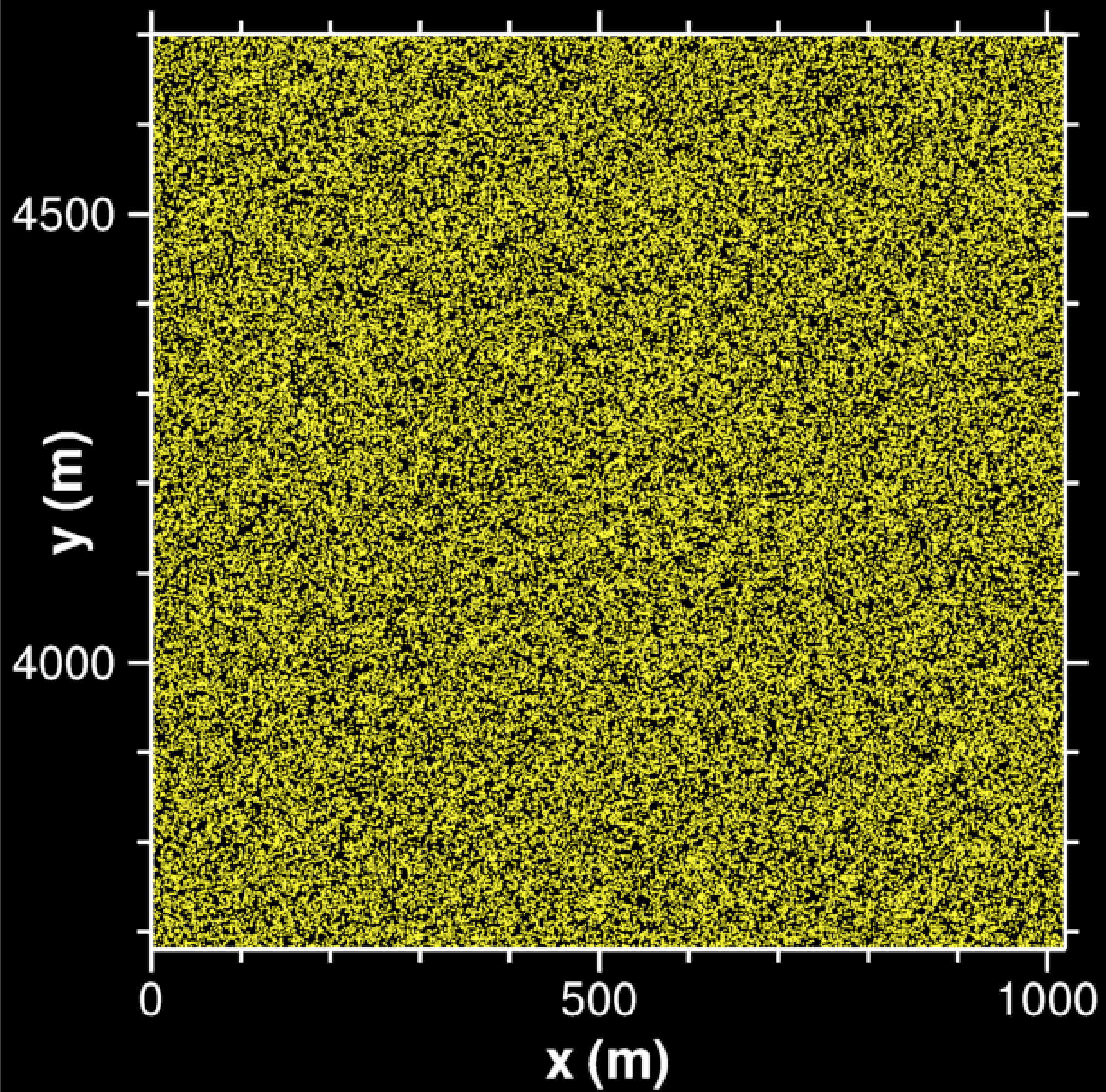
FREE CONVECTION 512^3 W-FIELD

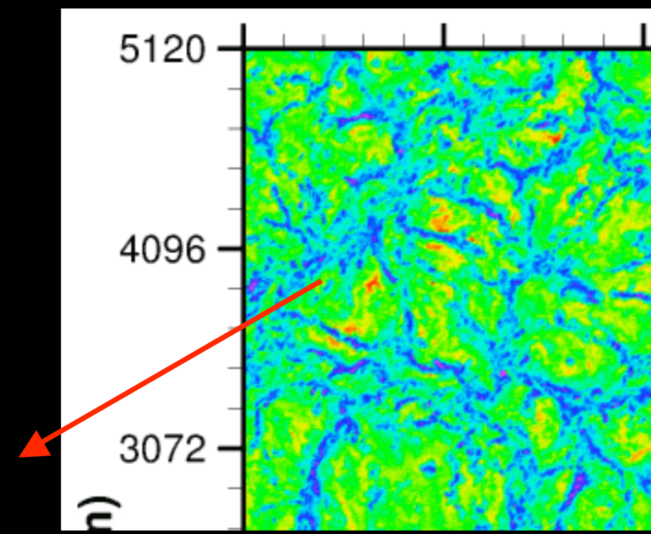


$$\triangle x = \triangle y = 10\ m$$

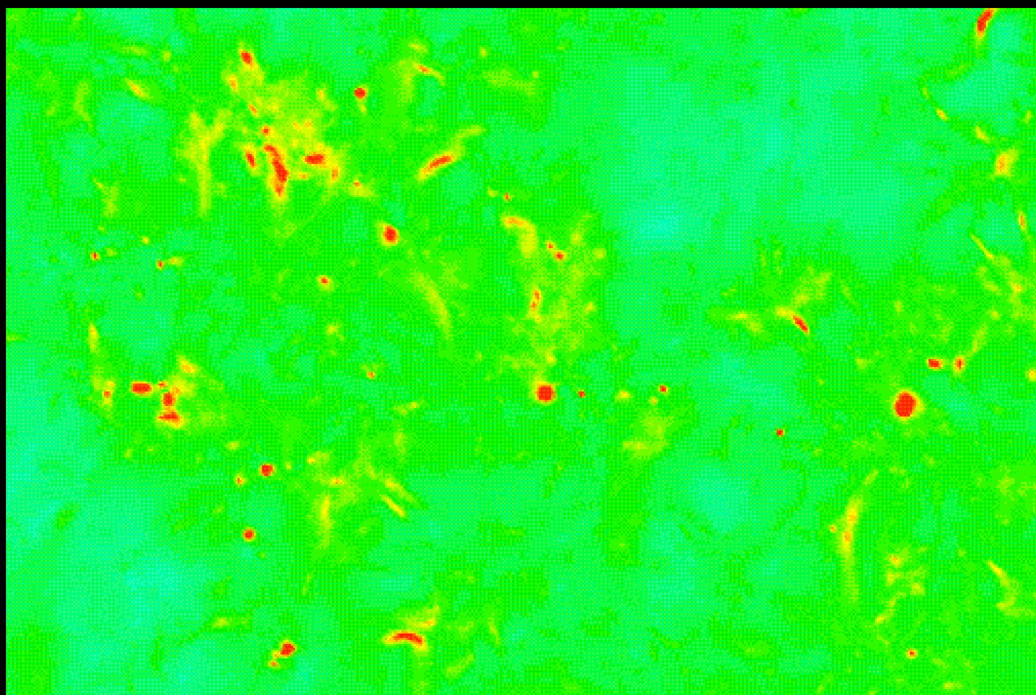
$$\triangle z = 4\ m$$

PARTICLE TRACING IN X-Y PLANE 1024^3 SIMULATION





TEMPORAL EVOLUTION OF VORTICES IDENTIFIED BY LOW (NEGATIVE) PRESSURE



$3800\ m$

$z = 24\ m$

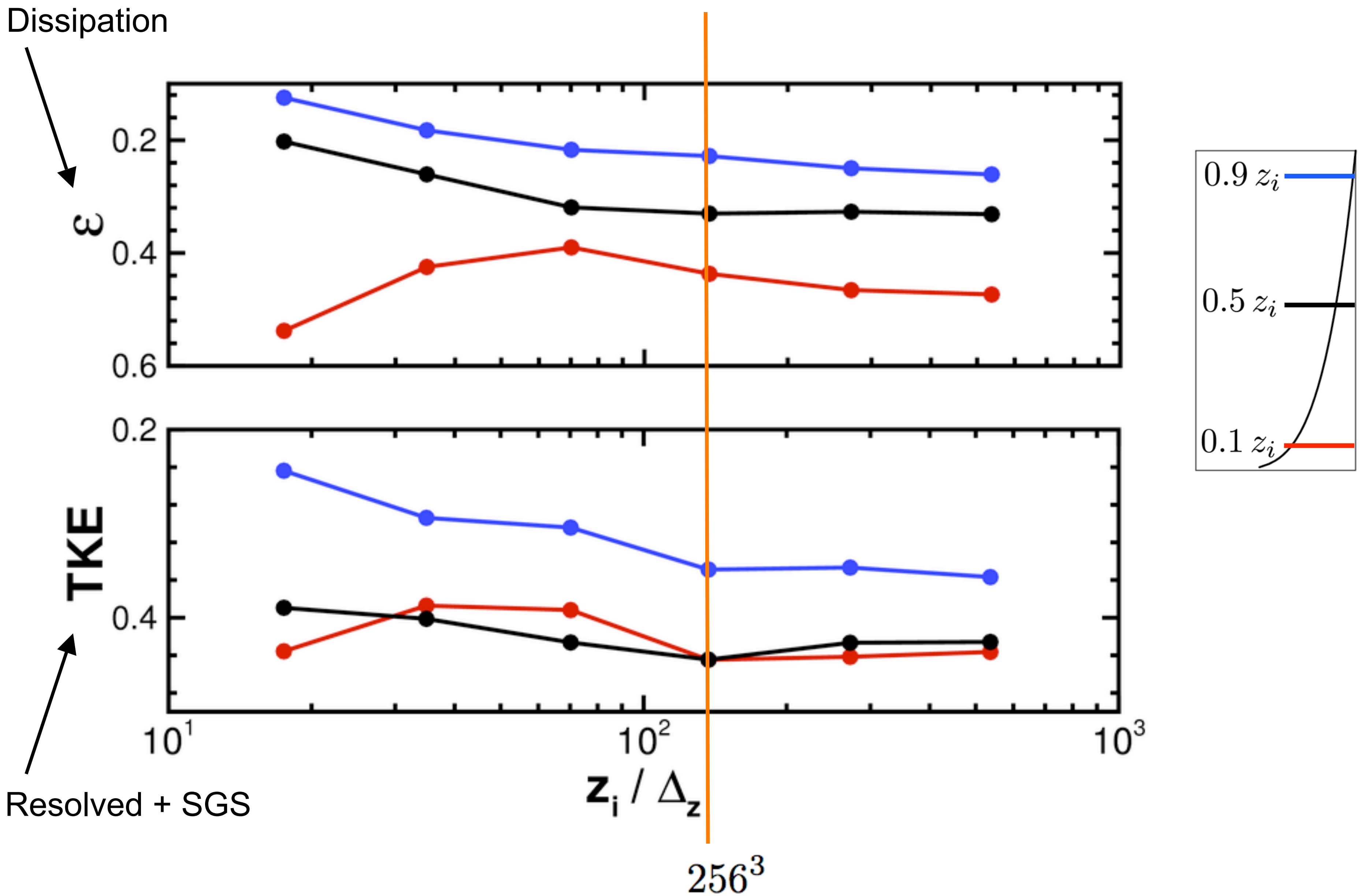
Dust devil image courtesy NASA

DO LES STATISTICS CONVERGE WITH MESH REFINEMENT?

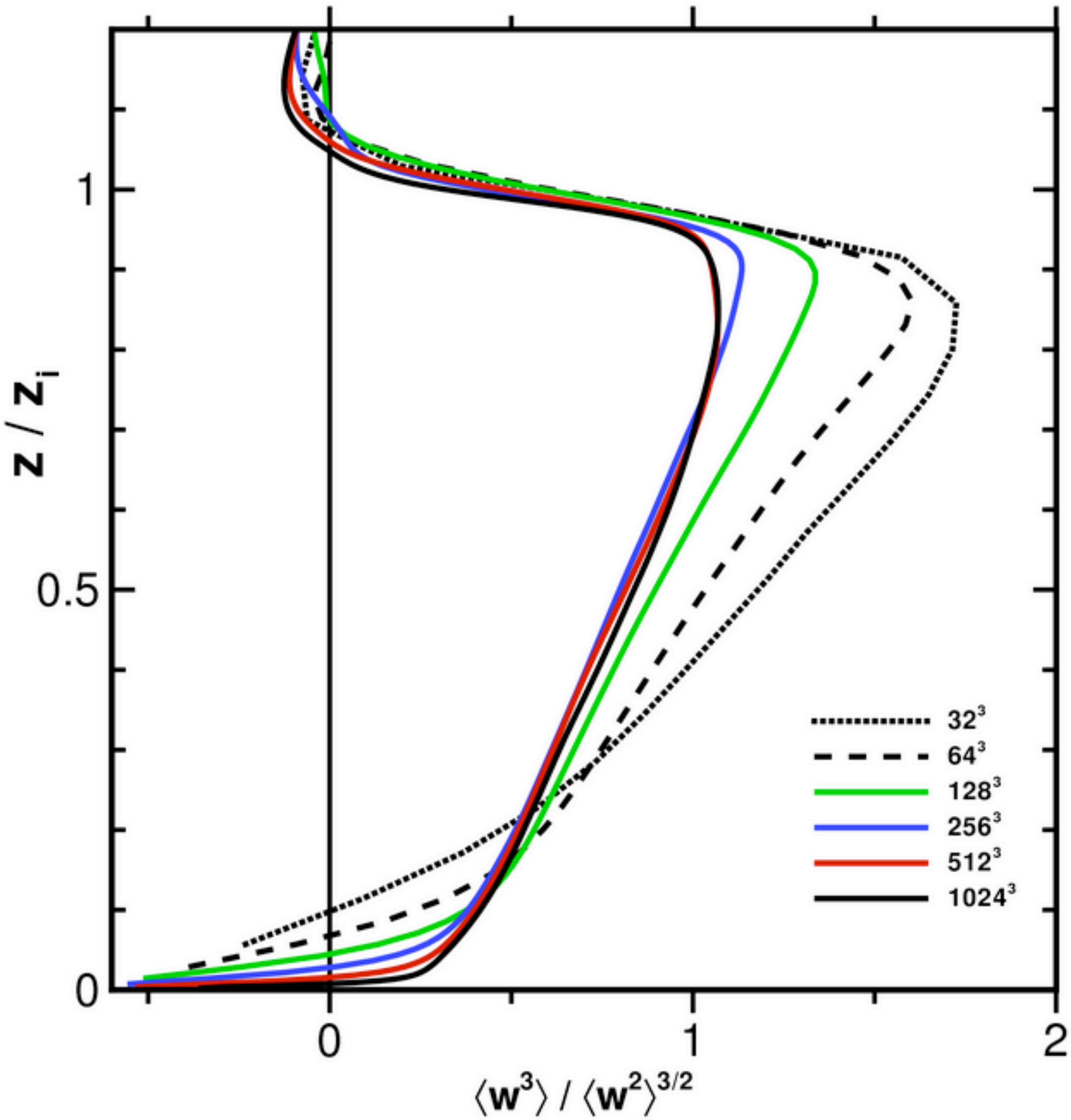
- LES DOMAIN: $(X_L, Y_L, Z_L) = (5120, 5120, 2048)$ m
- $\sim$ FREE CONVECTION
- STRONG INVERSION

Gridpoints	$\triangle x = \triangle y$ (m)	$\triangle z$ (m)	$z_i/\triangle z$	CPU (hrs)
32^3	160	64	17.5	0.3
64^3	80	32	34.9	3.5
128^3	40	16	70.2	58.6
256^3	20	8	137.0	971.0
512^3	10	4	272.0	11970.0
1024^3	5	2	536.7	~400000.0

DO LES STATISTICS CONVERGE WITH MESH REFINEMENT?



IMPACT OF GRID RESOLUTION ON SKEWNESS



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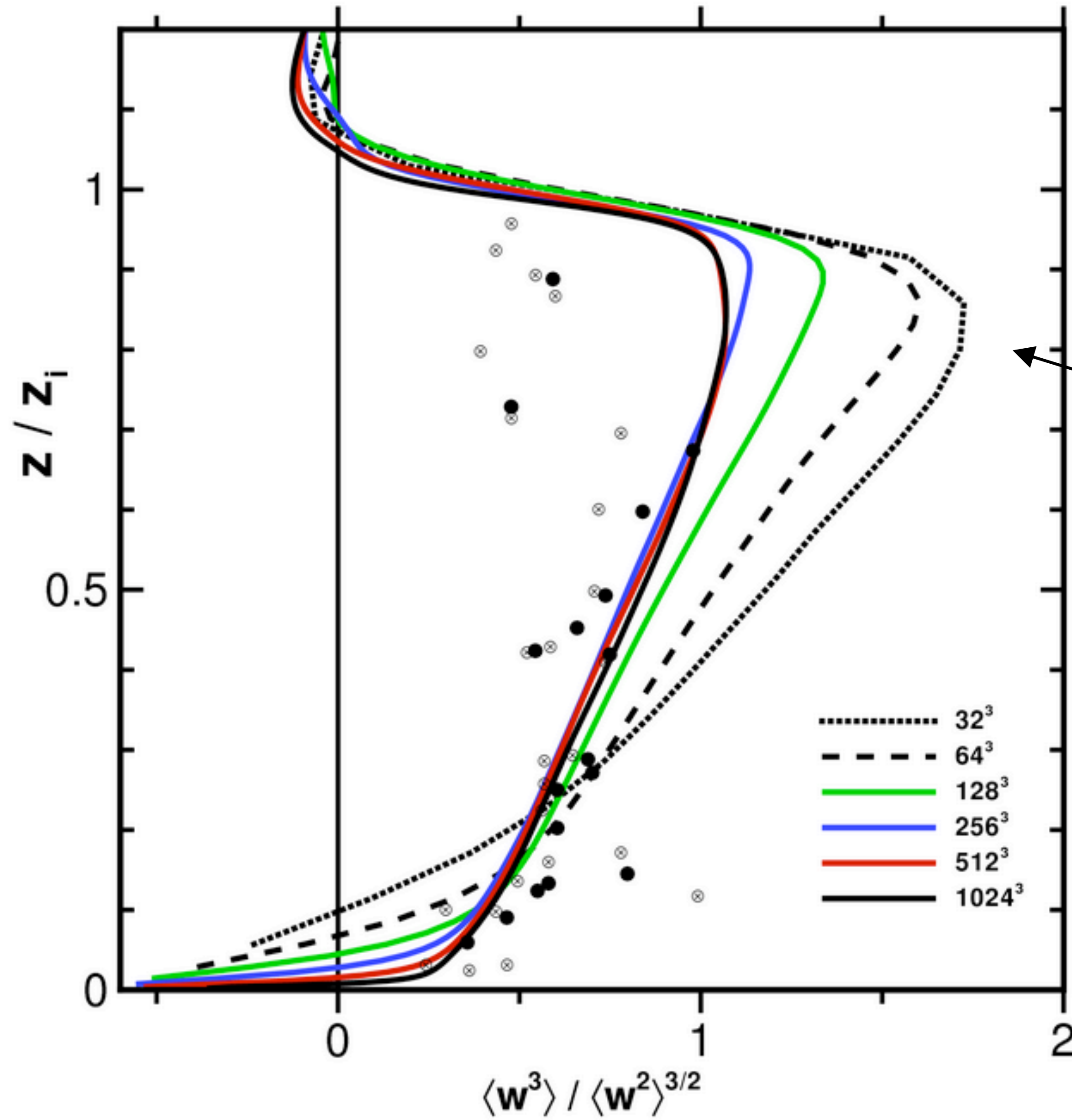


Small scales?
Inversion strength?
SGS model?

CONTRIBUTION OF SGS TO SKEWNESS

The *total* skewness is

$$S_w = \frac{\langle w^3 \rangle}{\langle w^2 \rangle^{3/2}}$$

Introduce SGS third and second order moments

$$\phi = \overline{w^3} - \overline{w}^3 \equiv \overline{www} - \overline{w}\,\overline{w}\,\overline{w}$$

$$\psi = \overline{w^2} - \overline{w}^2 \equiv \overline{ww} - \overline{w}\,\overline{w}$$

Total skewness in terms of resolved and SGS fields

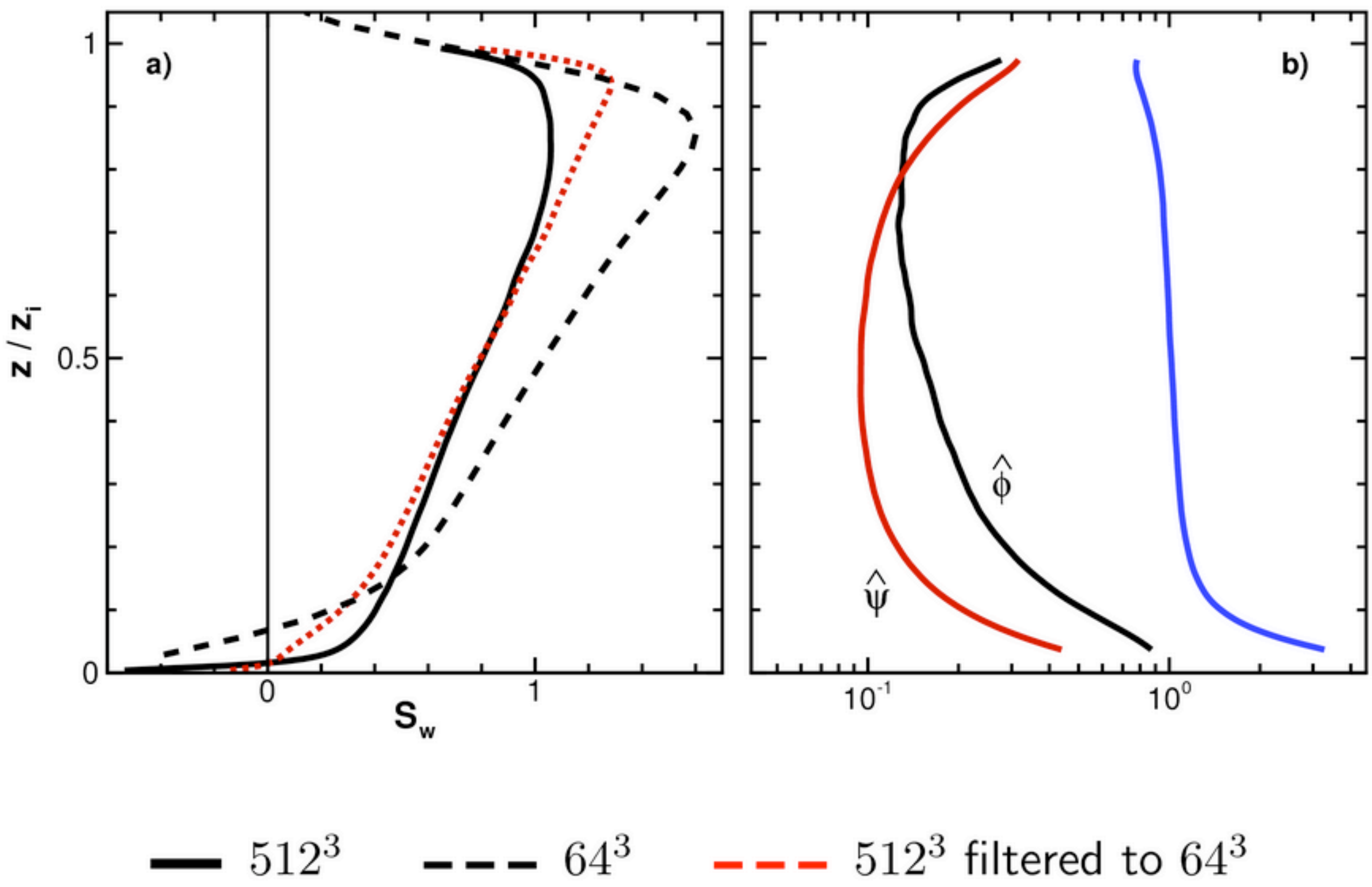
$$S_w = S_{\overline{w}} \frac{(1-\hat{\psi})^{3/2}}{(1-\hat{\phi})}$$

Total

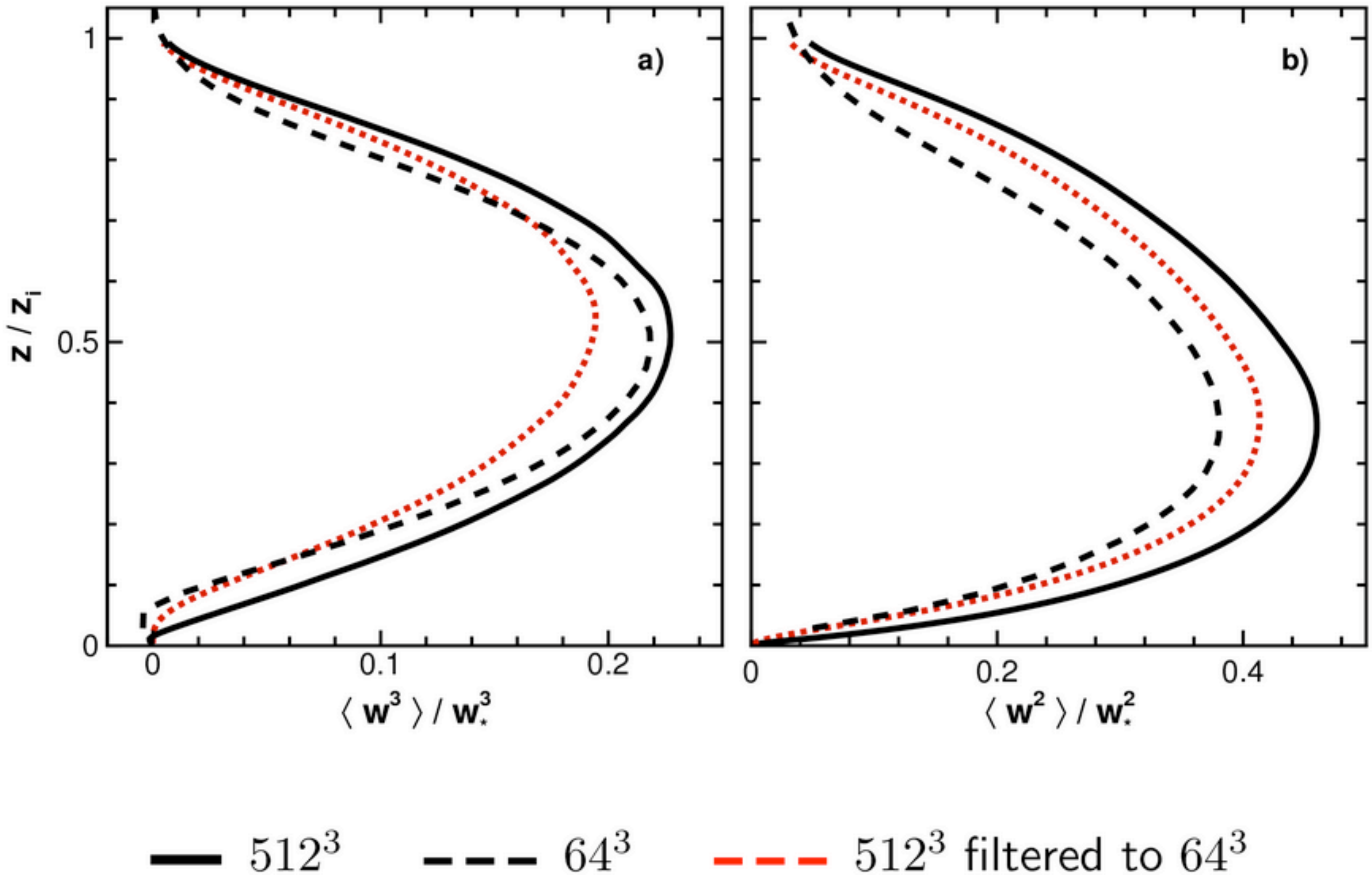
Resolved

SGS correction

FILTERED SKEWNESS AND SGS MOMENTS



VERTICAL VELOCITY MOMENTS



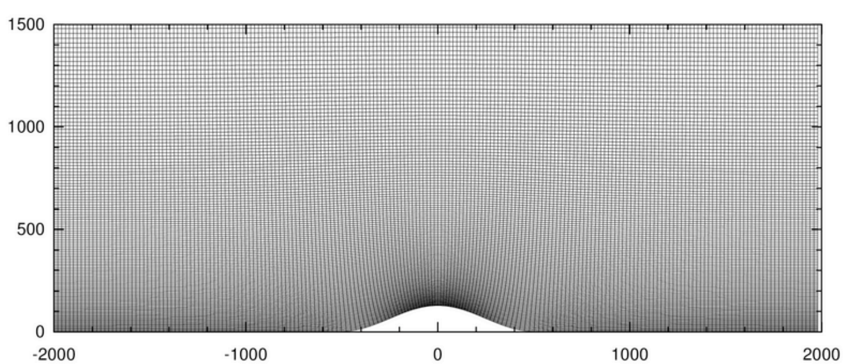
HOW ABOUT SIMPLE TERRAIN?

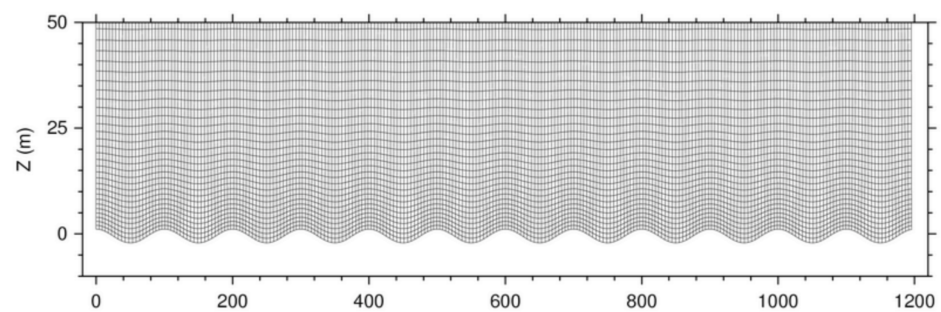
LES FOR FLOW OVER HILLS AND WAVES

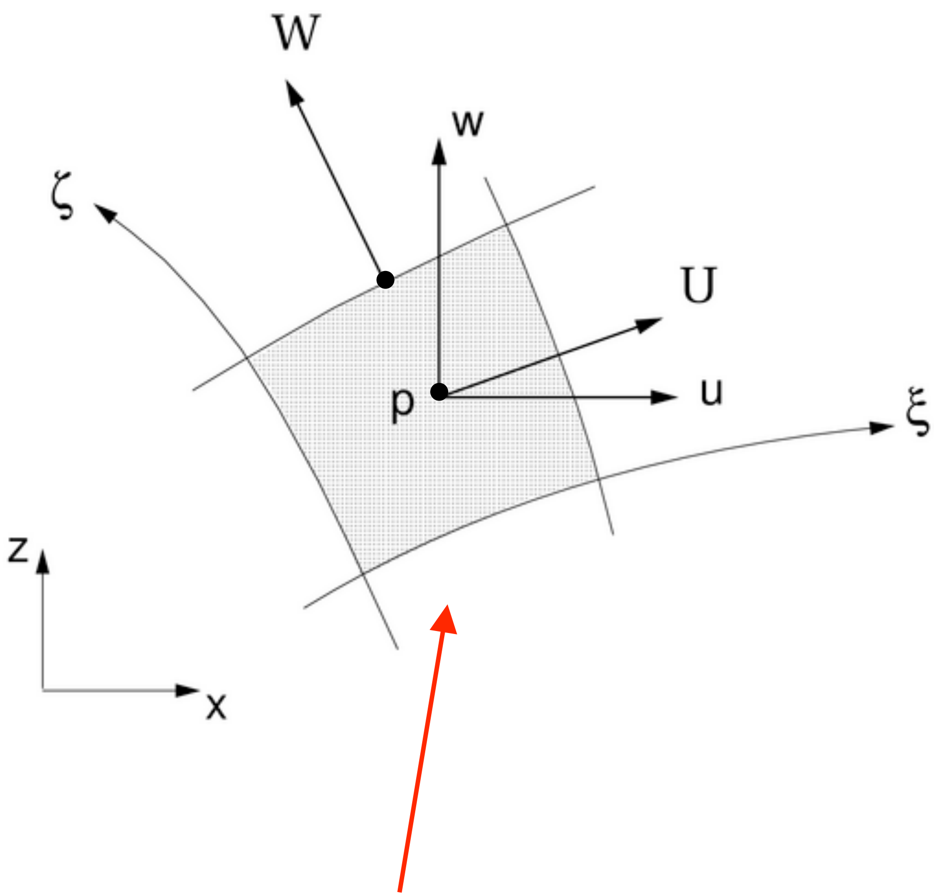
Orography in LES:

- Approaches are:
  - Cast equations in surface fitted coordinates $x_i \Rightarrow \xi_i$
  - Unstructured meshes, Immersed boundaries, Wavelet techniques

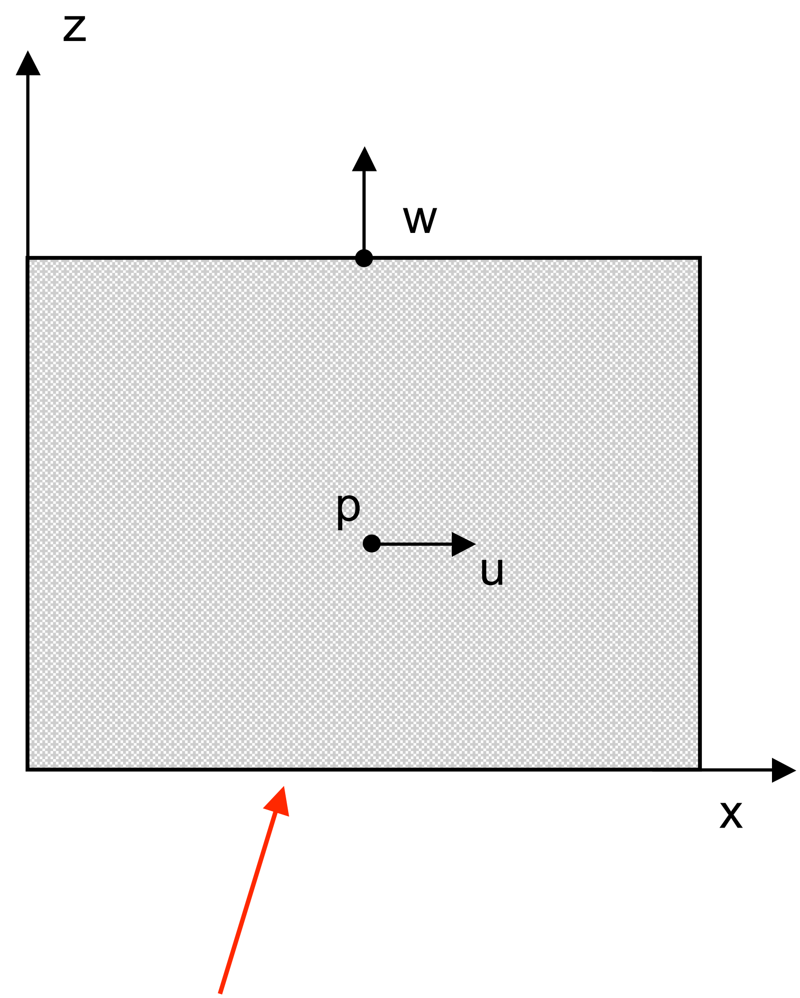
- Including orography in "LES" is a research topic
  - High-Re with "z_o" boundary conditions
  - Filtering when the mesh varies considerably, $e.g.$, commutation errors, ...
  - SGS models in complex flows







Co-located scheme



Vertically staggered scheme

SURFACE FITTED CO-LOCATED METHOD

Attributes:

- Simple compact stencil
- Use contra-variant "flux" velocities U_i in formulating the LES equations
- Trick is to use "momentum-interpolation" of the right-hand sides Zang *et al.*(1994), Sullivan *et al.*(2000), Sullivan *et al.*(2008)
- Maintains strong velocity-pressure coupling

Outline of the equations:

$$\frac{\partial U_i}{\partial \xi_i} = 0$$

$$\frac{\partial}{\partial t}\left(\frac{u_i}{J}\right) + \frac{\partial}{\partial \xi_j} U_j u_i = \mathcal{R}_i$$

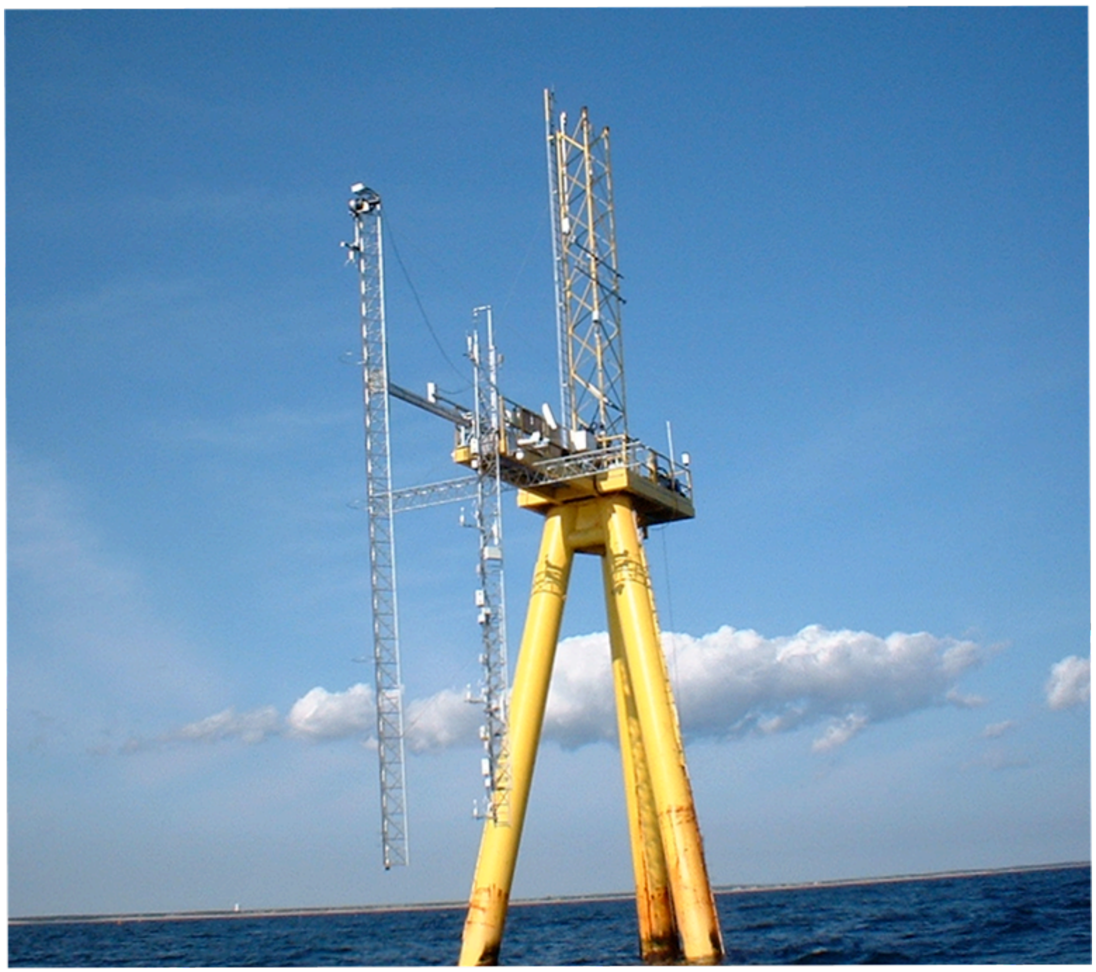
$$\frac{\partial}{\partial \xi_i}\left[\frac{1}{J}\frac{\partial \xi_i}{\partial x_j}\frac{\partial \xi_m}{\partial x_j}\frac{\partial p^*}{\partial \xi_m}\right] = \mathcal{S}$$

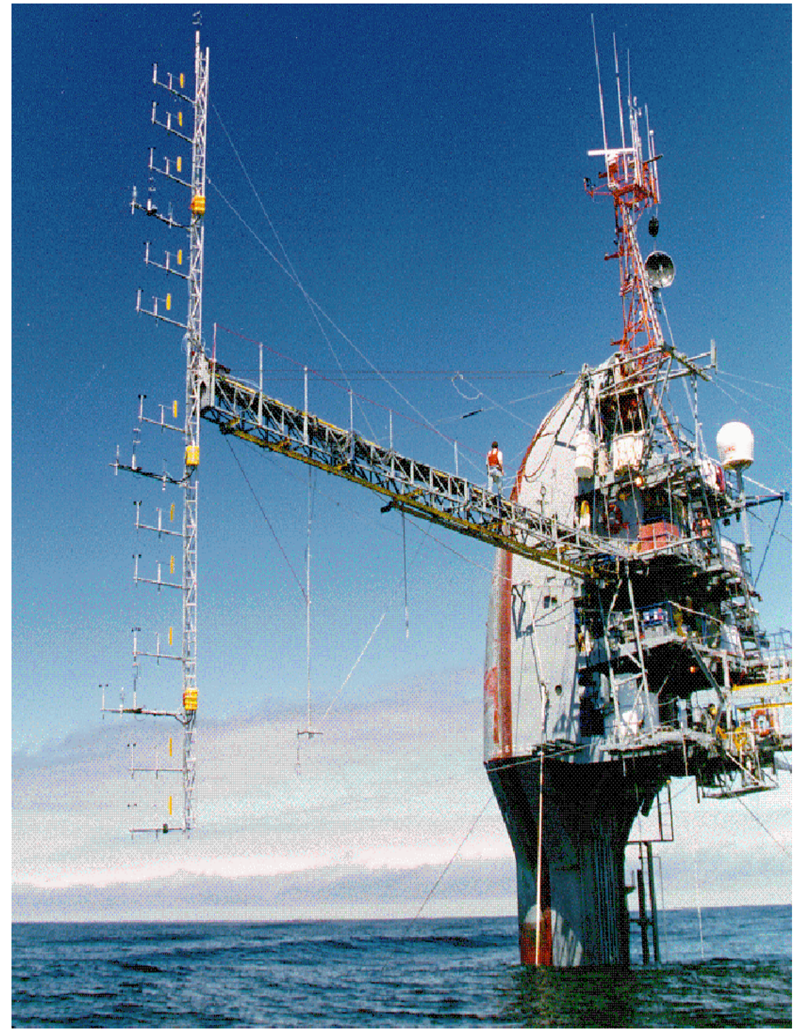
General elliptic equation

WHAT CAN USE IT FOR?

OBSERVATIONS OF WINDS AND WAVES

Air-Sea Interaction Tower near Martha's Vineyard during CBLAST





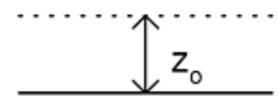
FLIP deployed off the California coast during MBL II

WAVE-WIND LES EXPERIMENTS

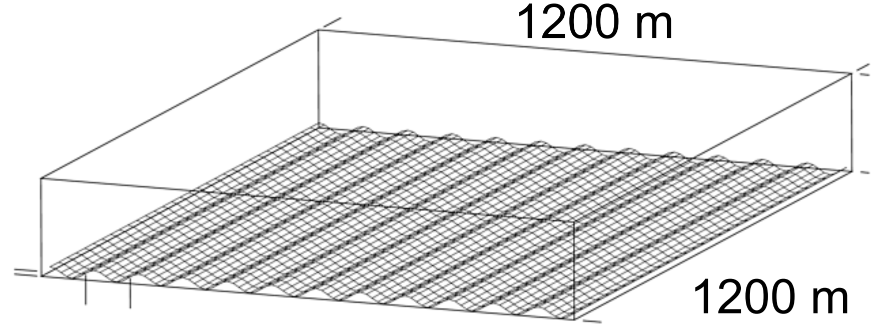
Forcing (U_g, V_g) (m/s)	Wind-wave Angle ϕ (degrees)	Wave Age
(5,0)	≈ 6.8	no waves
(5,0)	≈ 19	bumps
(5,0)	≈ -2.3	> 2
(2,0)	≈ -6.1	> 4
(5,5)	≈ 45	> 2
(-5,0)	≈ 180	> 2
(-5,5)	≈ 135	> 2
(12.5,0)	≈ 0	bumps
(12.5,0)	≈ 0	bumps + heating
(12.5,0)	≈ 0	≈ 1

c =12.5m/s, ak =0.1, a =1.6m, λ =100m, z_o =0.0002m

Parameterized surface roughness



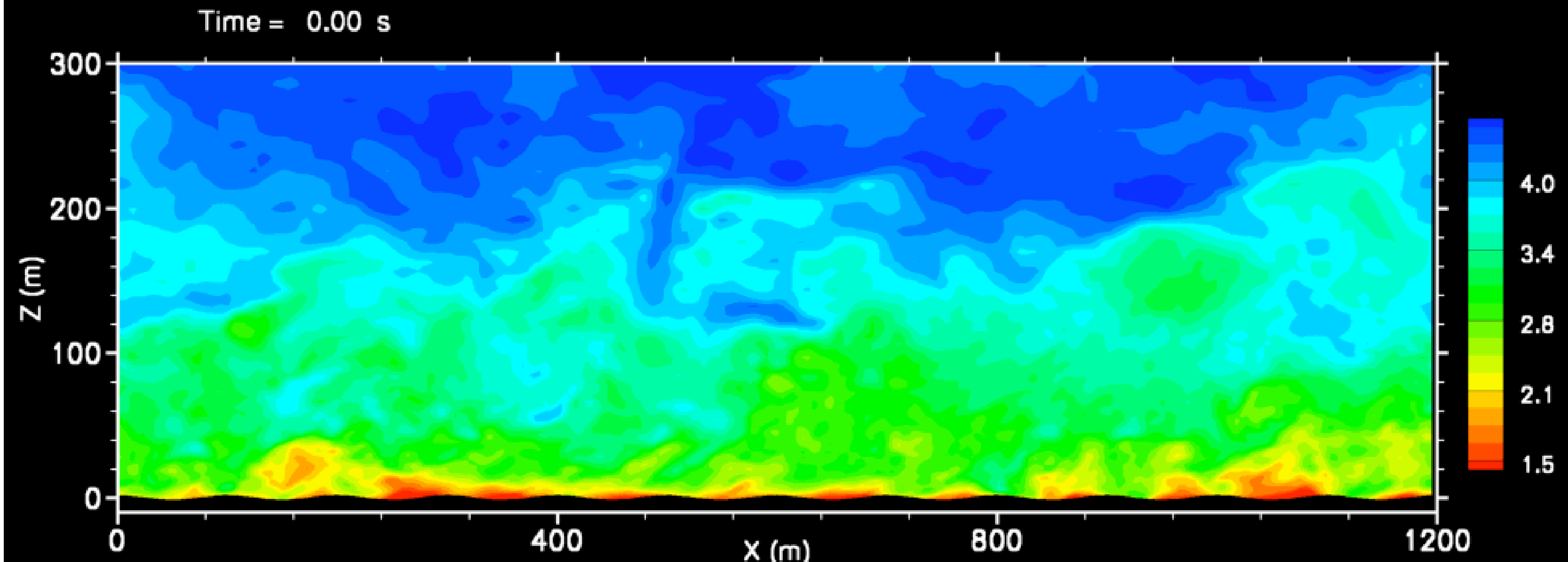
Parameterized z_o+ resolved wave



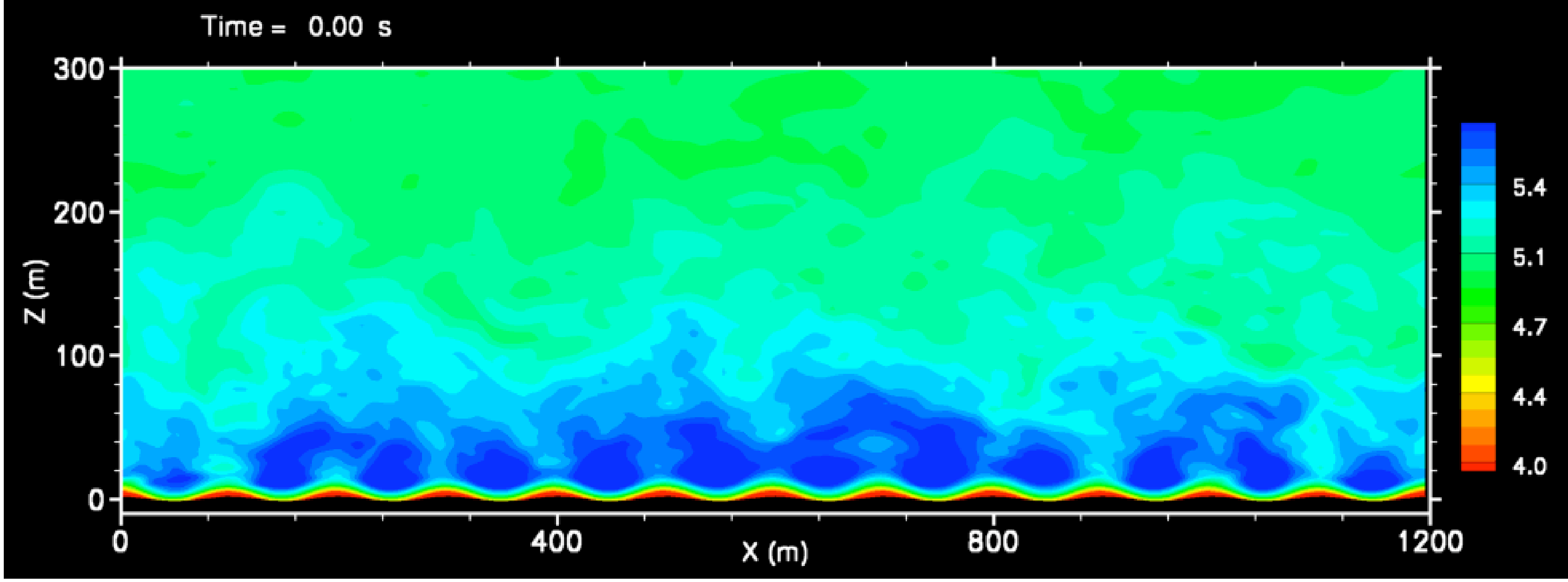
TURBULENT FLOW IN THE PBL ABOVE WAVES

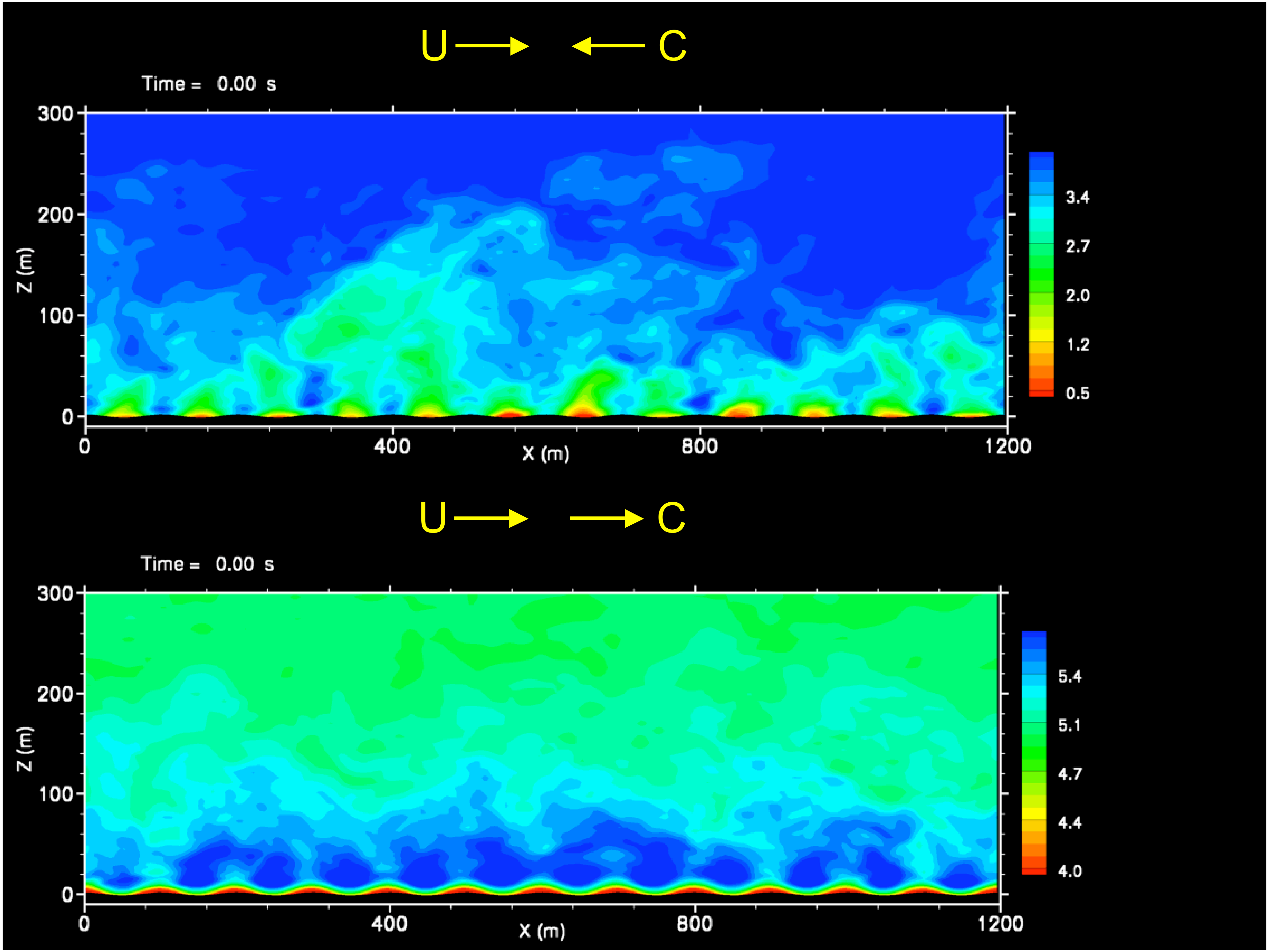
U-contours

HILLS

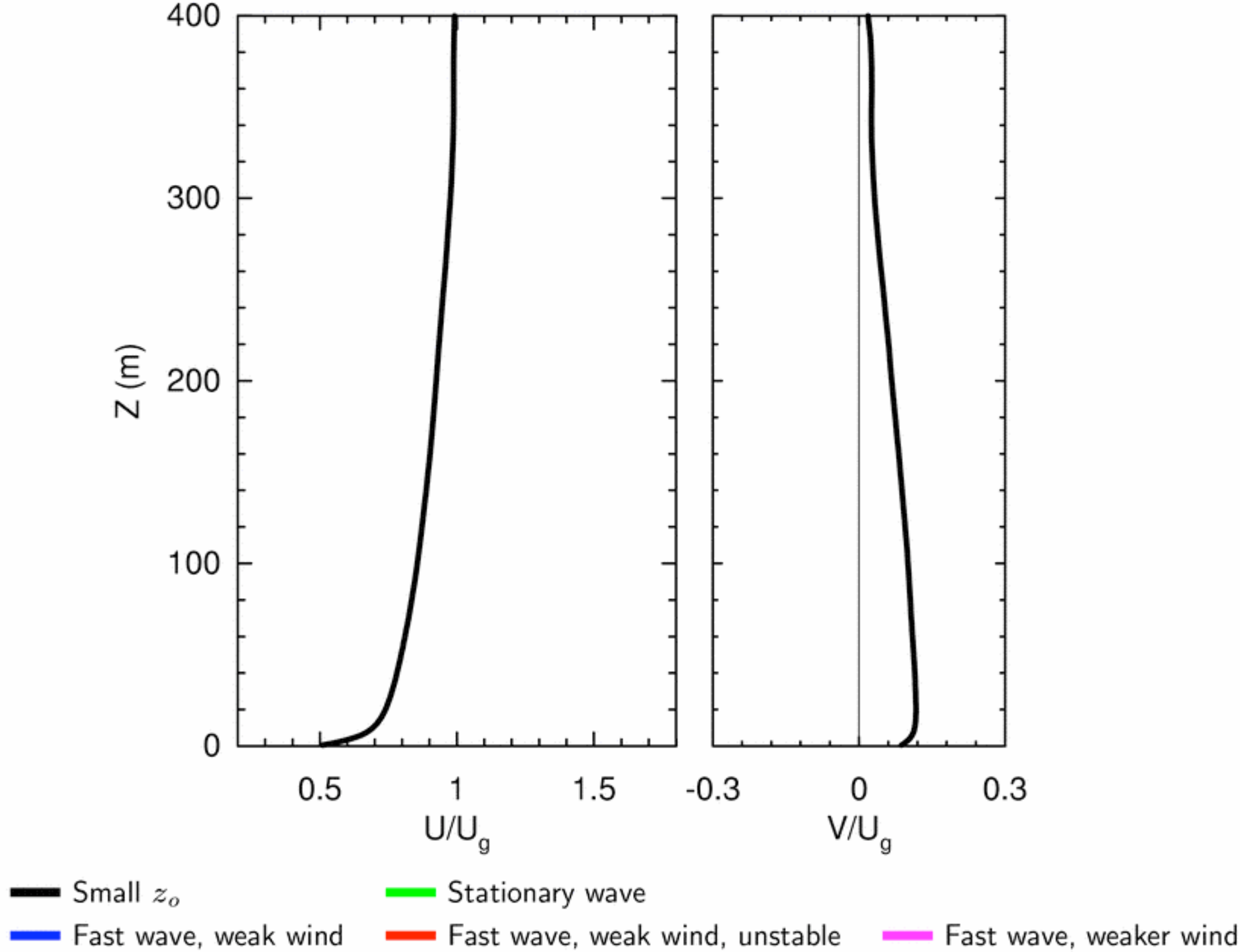


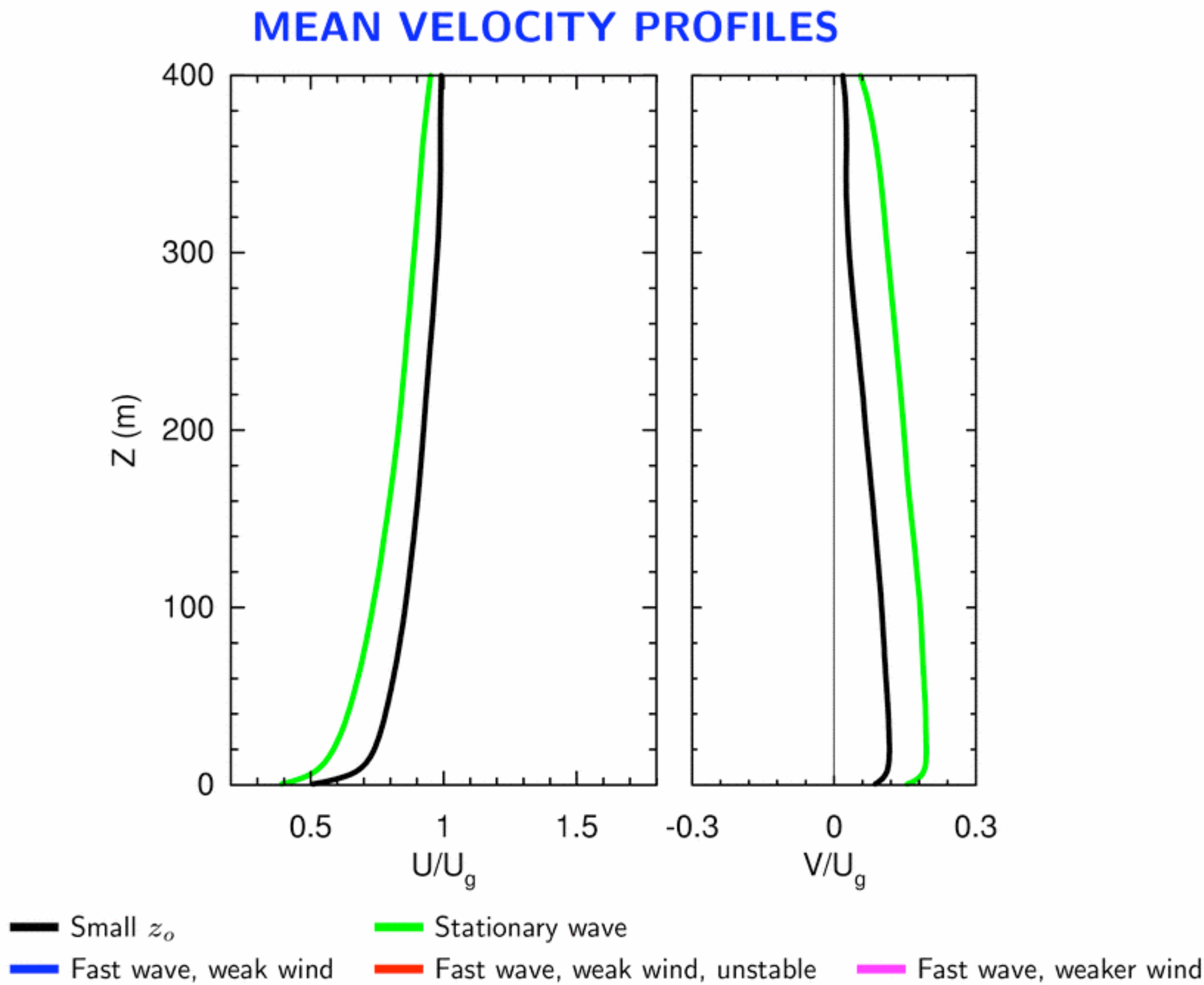
SWELL



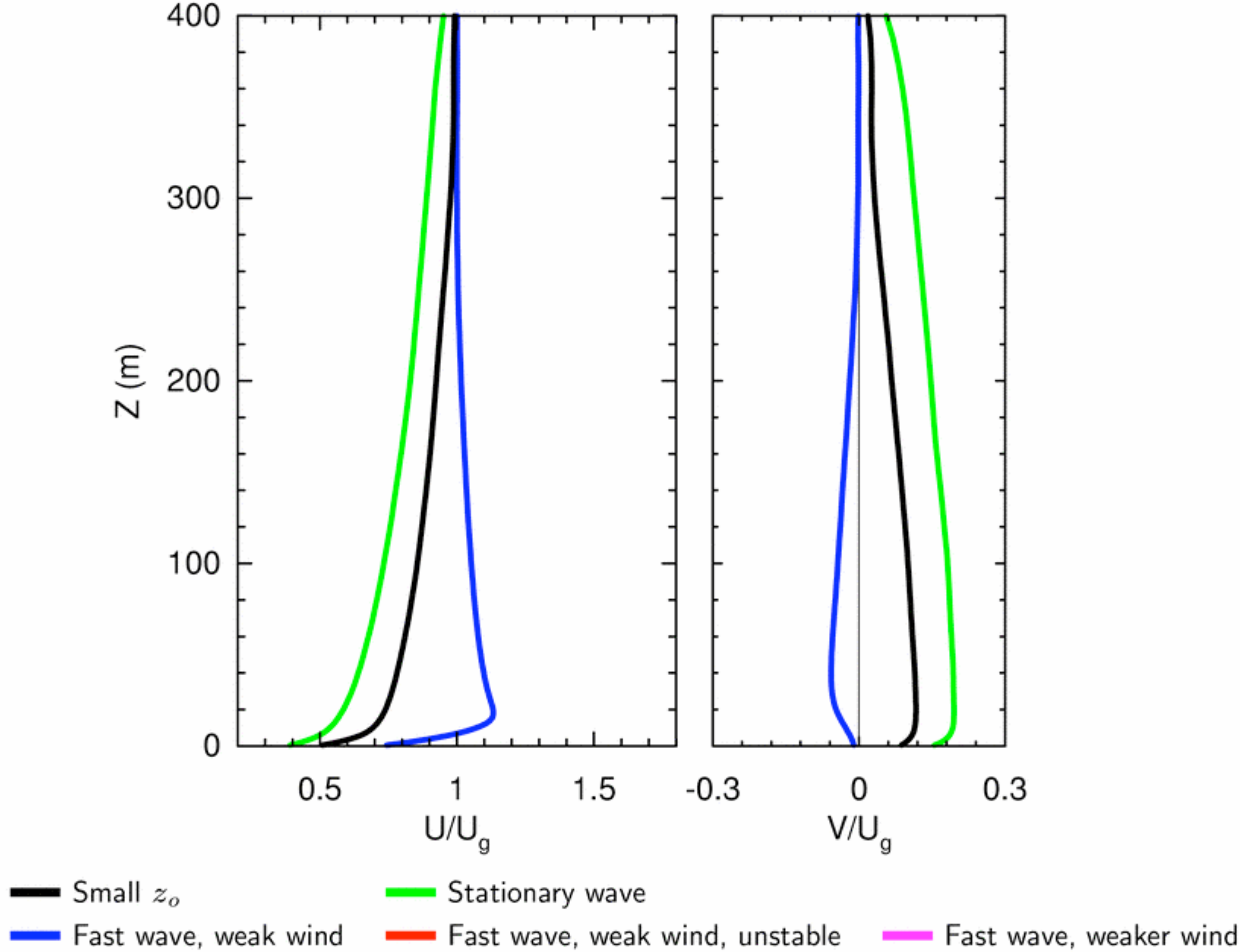

U → ← C
Time = 0.00 s
300
200
100
0
Z (m)
0
400
800
1200
X (m)
3.4
2.7
2.0
1.2
0.5
U → → C
Time = 0.00 s
300
200
100
0
Z (m)
0
400
800
1200
X (m)
5.4
5.1
4.7
4.4
4.0

MEAN VELOCITY PROFILES




MEAN VELOCITY PROFILES
Z (m)
400
300
200
100
0
0.5
1
1.5
U/U$_g$
-0.3
0
0.3
V/U$_g$
Small z_o
Stationary wave
Fast wave, weak wind
Fast wave, weak wind, unstable
Fast wave, weaker wind

MEAN VELOCITY PROFILES



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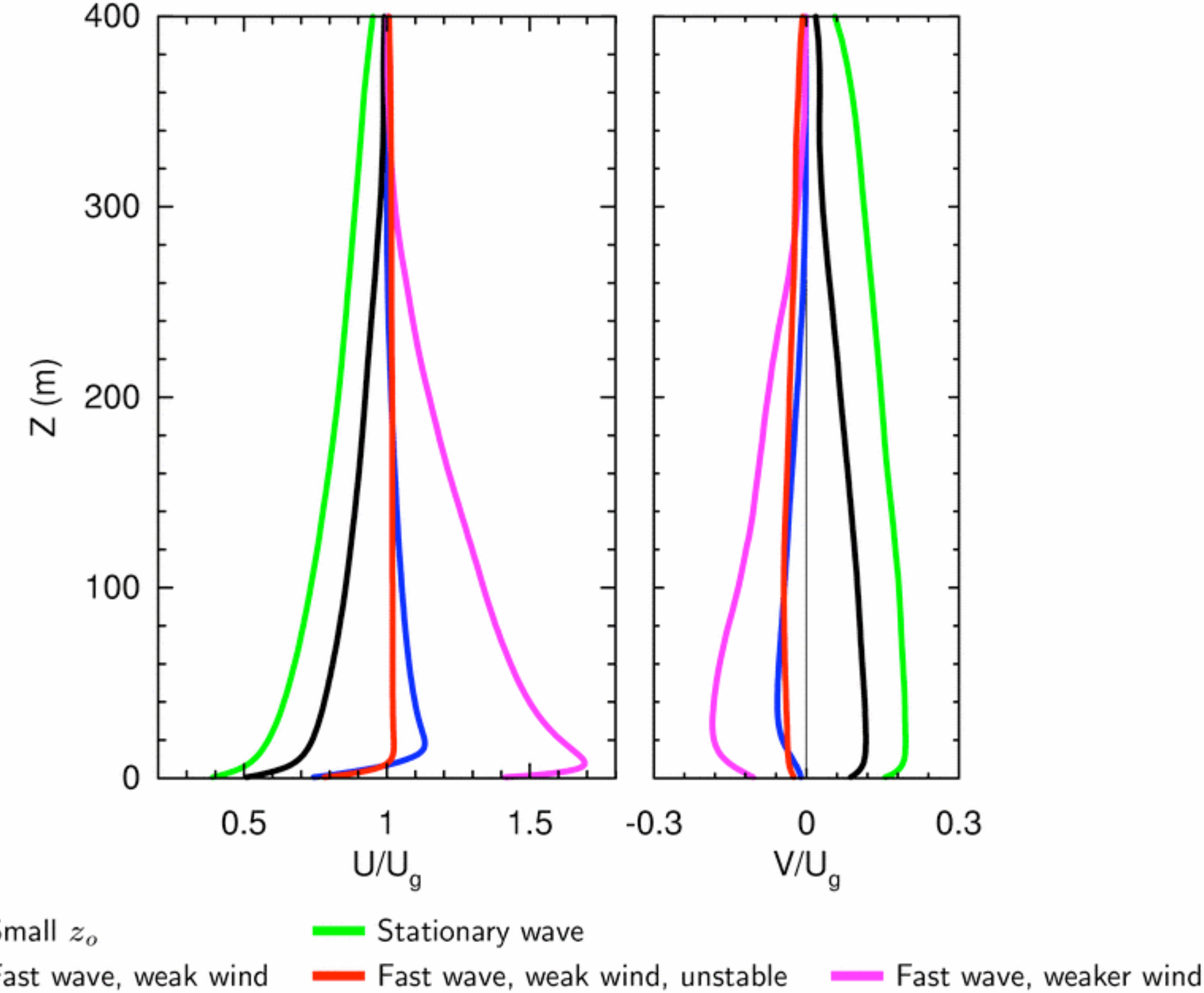
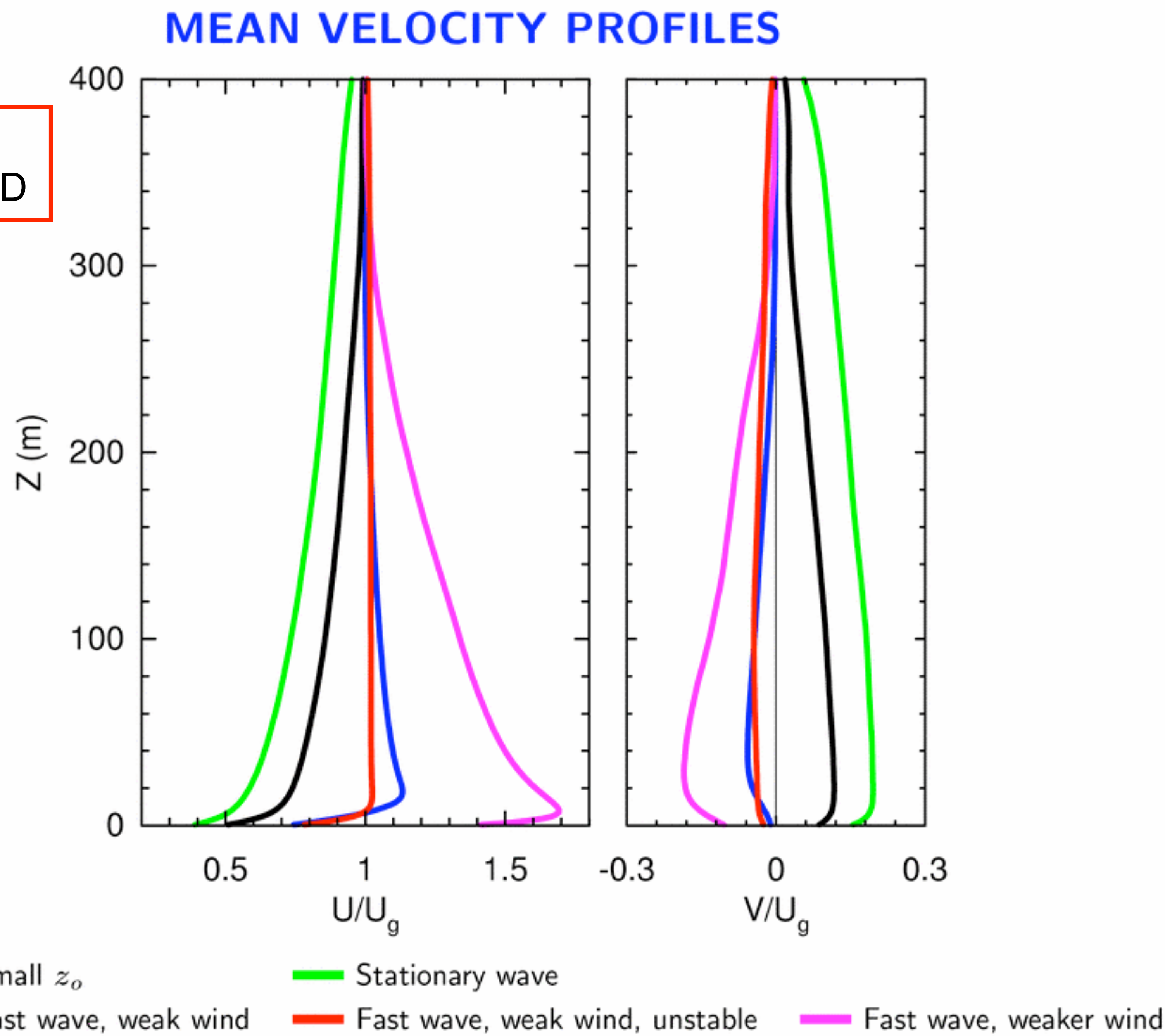
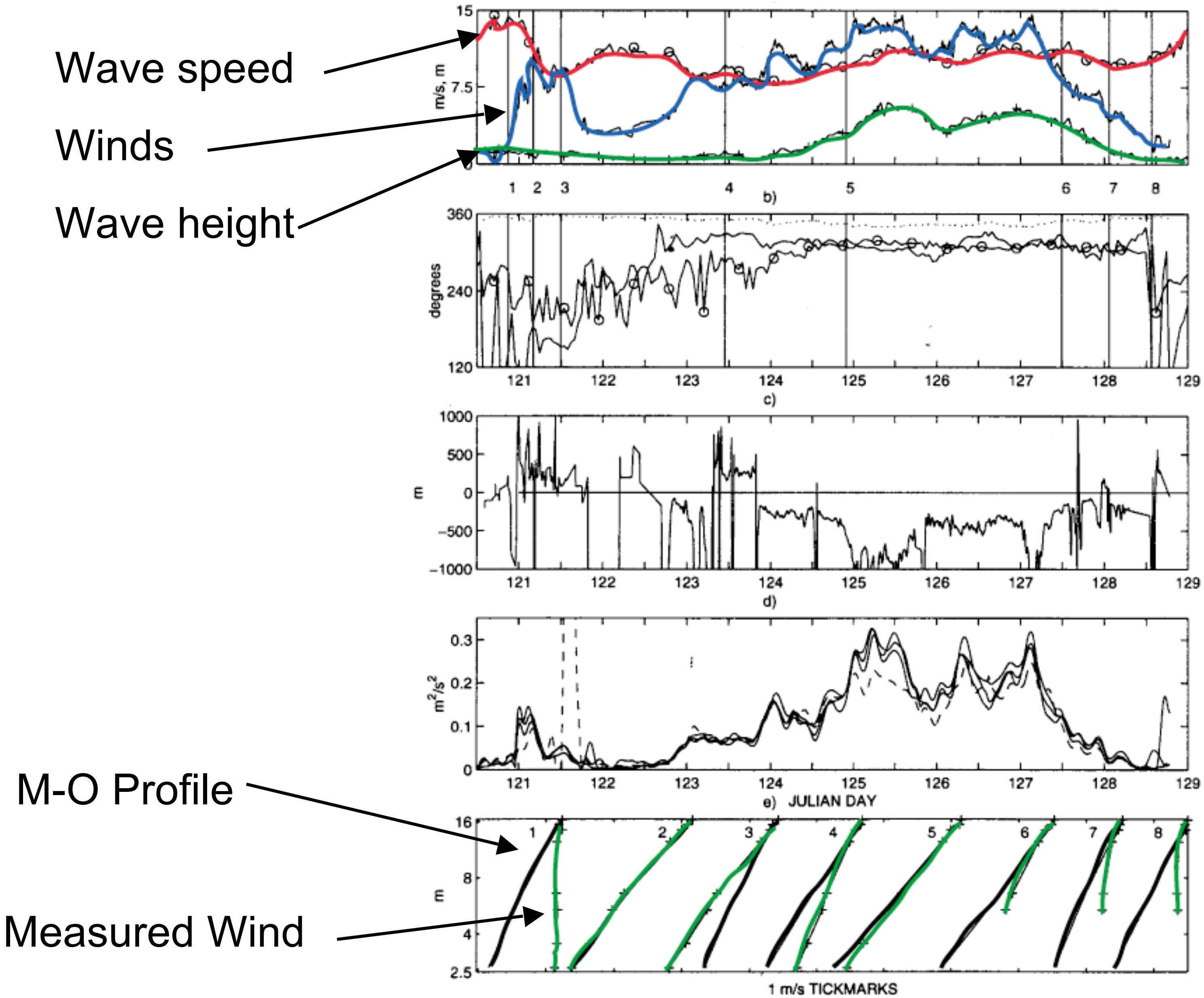


WAVE-
DRIVEN WIND

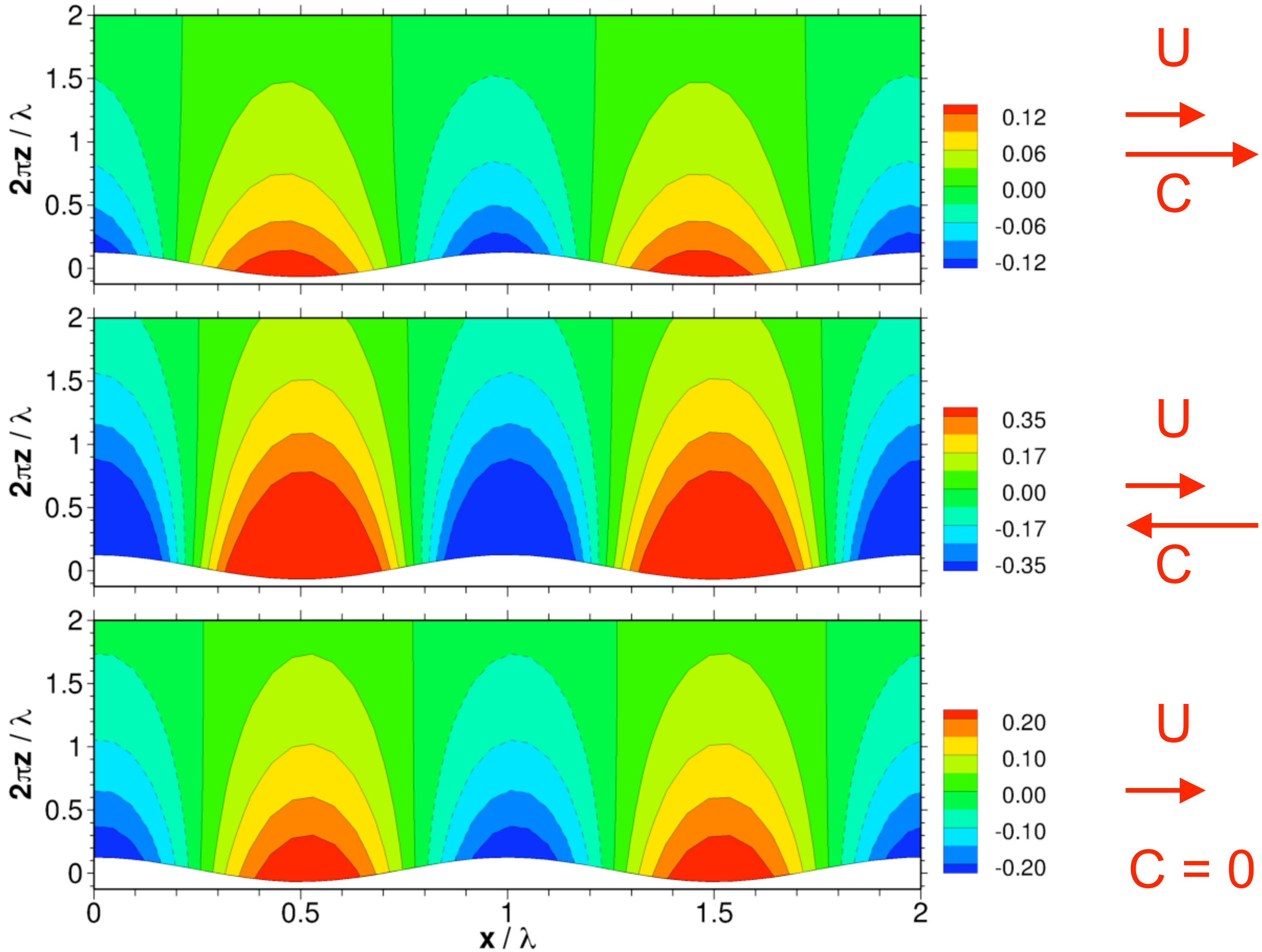


MBL II (FLIP) OBSERVATIONS

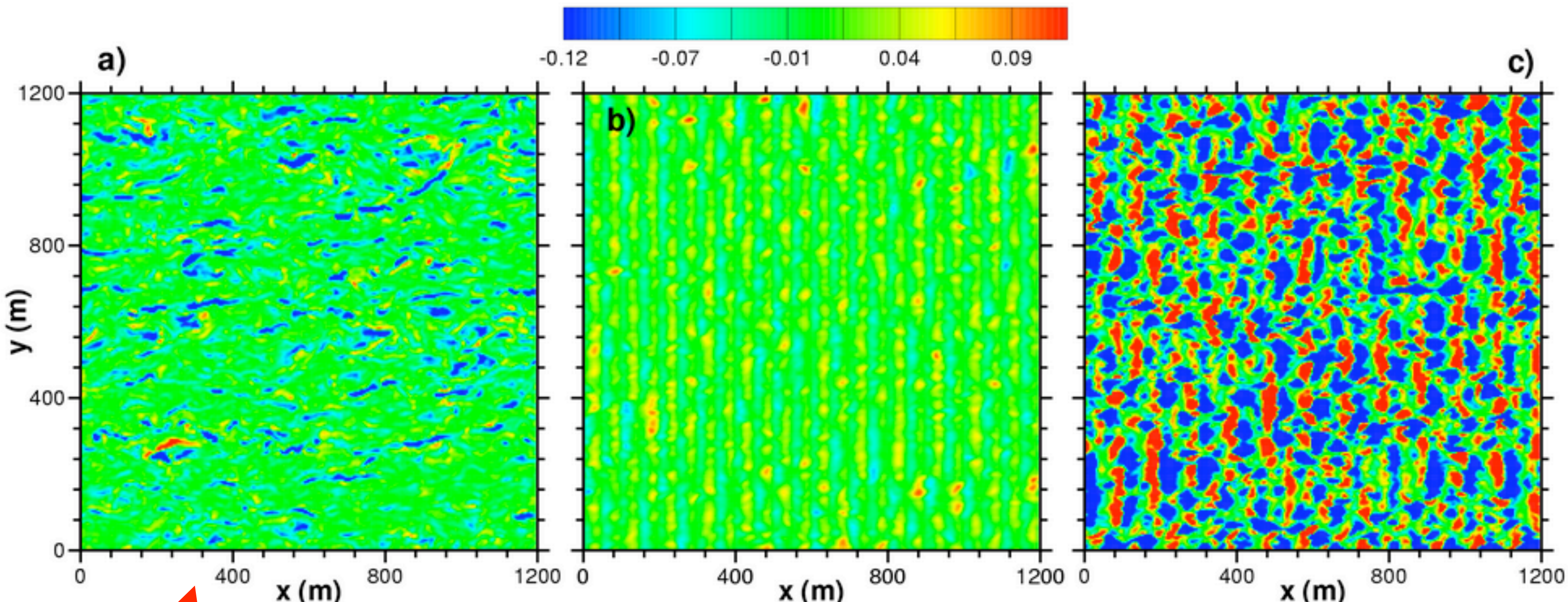


Data from S. Miller

PHASE AVERAGED PRESSURE FIELD FOR VARYING WAVE AGE



MOMENTUM FLUX $U'W'$ IN $X - Y$ PLANES (Z = 20m)



No waves,
z_o surface

$$\langle u'w' \rangle < 0$$

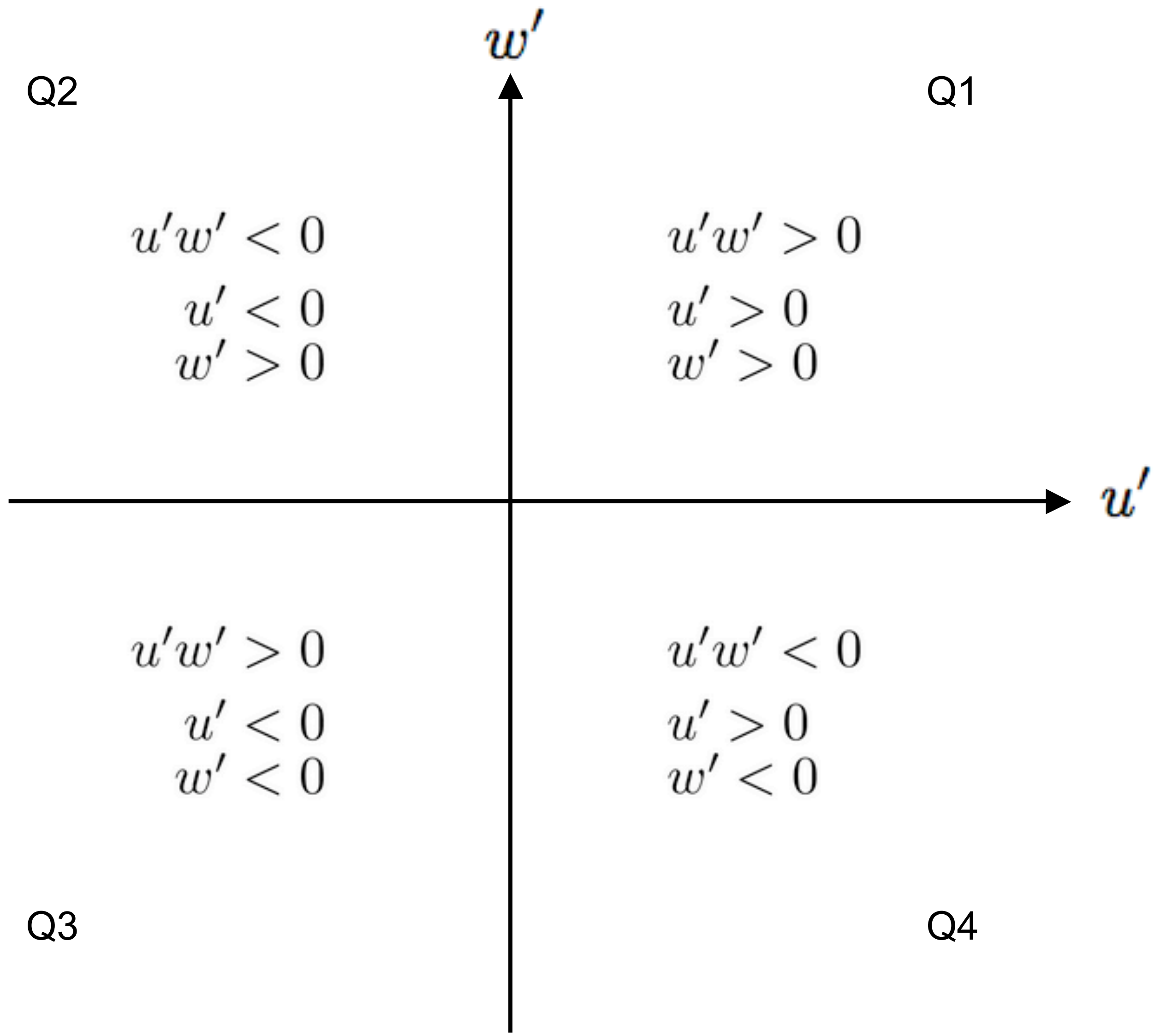
Resolved swell
leading the wind

$$\langle u'w' \rangle \approx 0$$

Resolved swell
opposing the wind

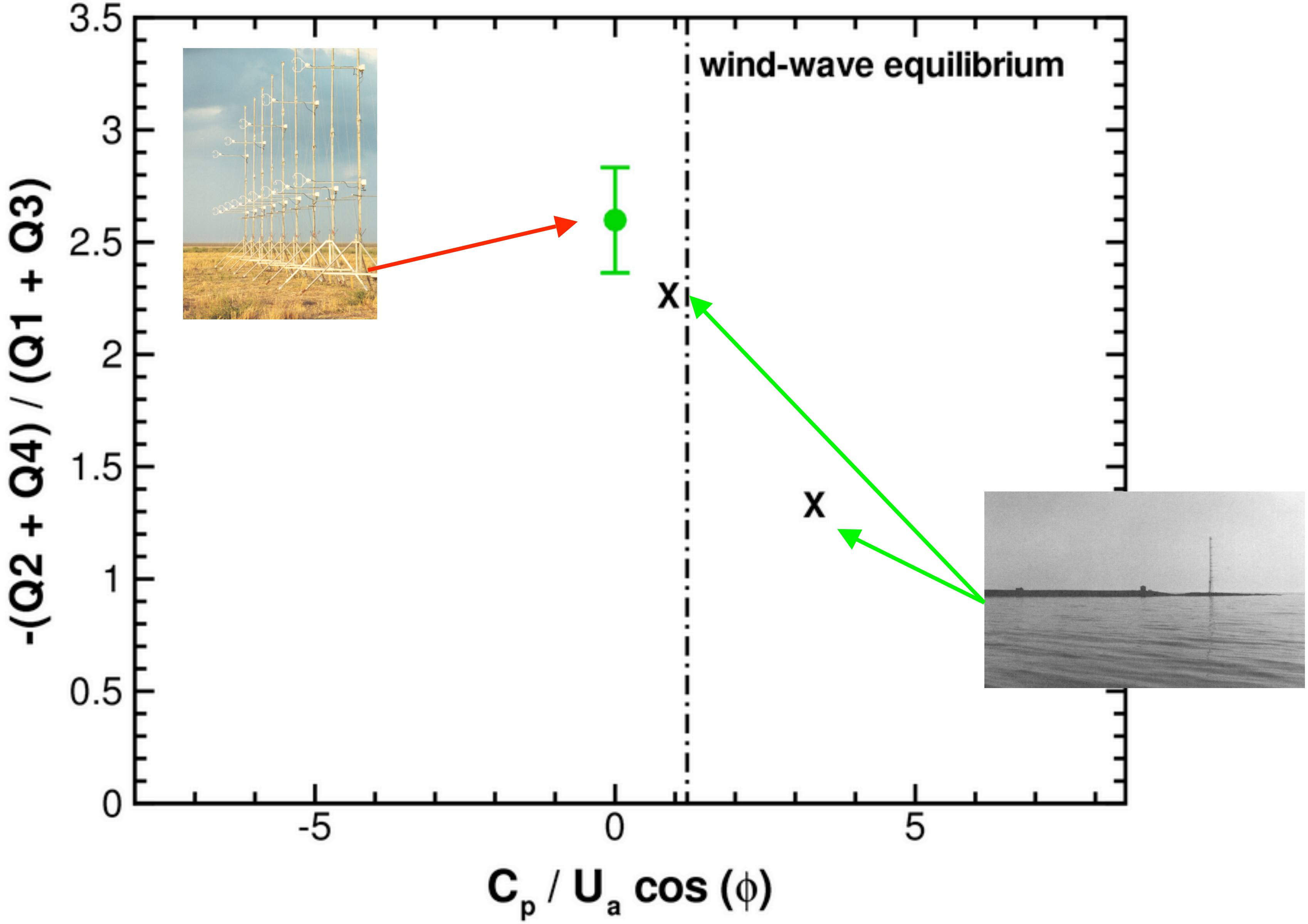
$$\langle u'w' \rangle << 0$$

QUADRANT ANALYSIS OF MOMENTUM FLUX

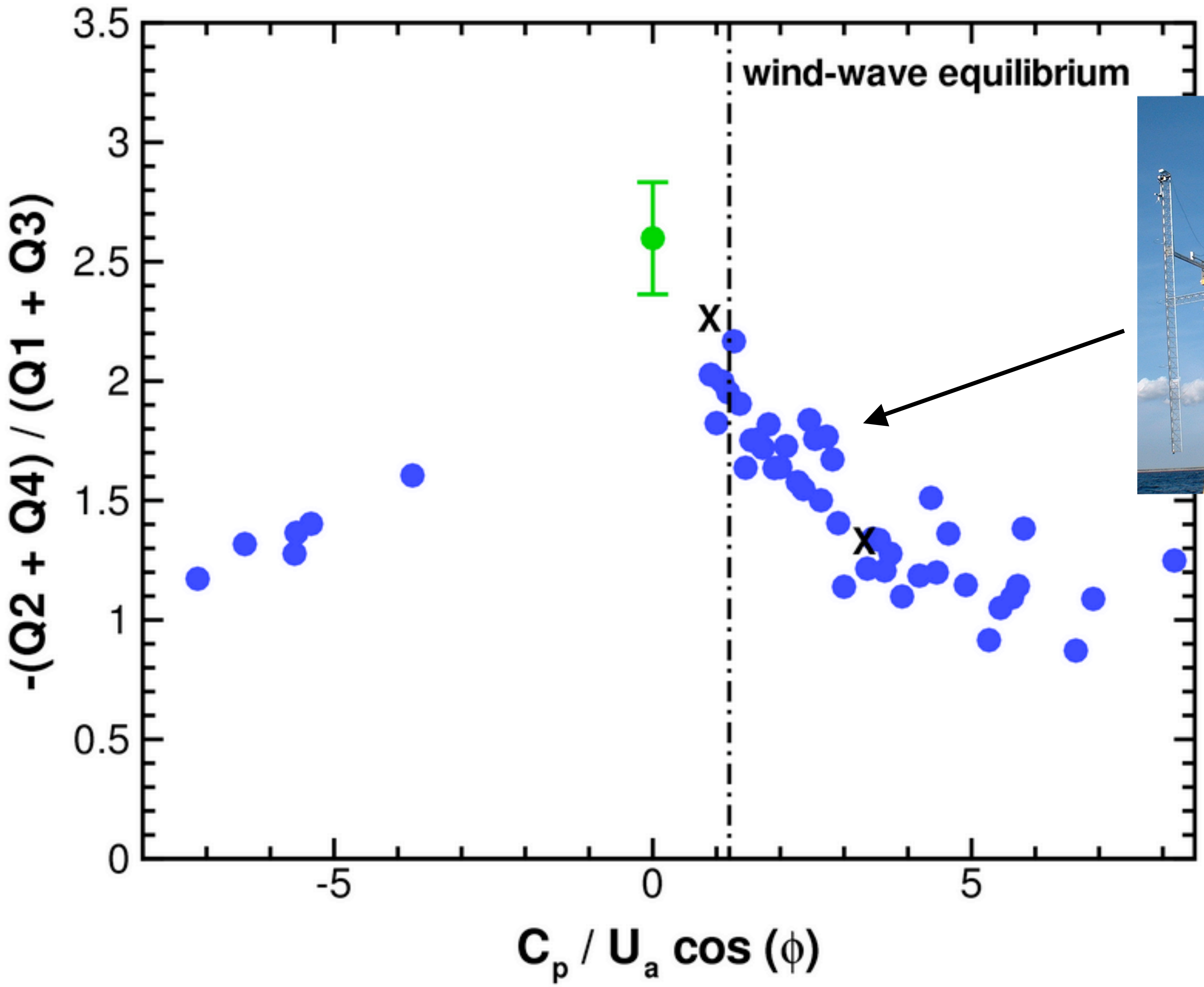


Ratio = -(Q2 + Q4)/(Q1 + Q3)

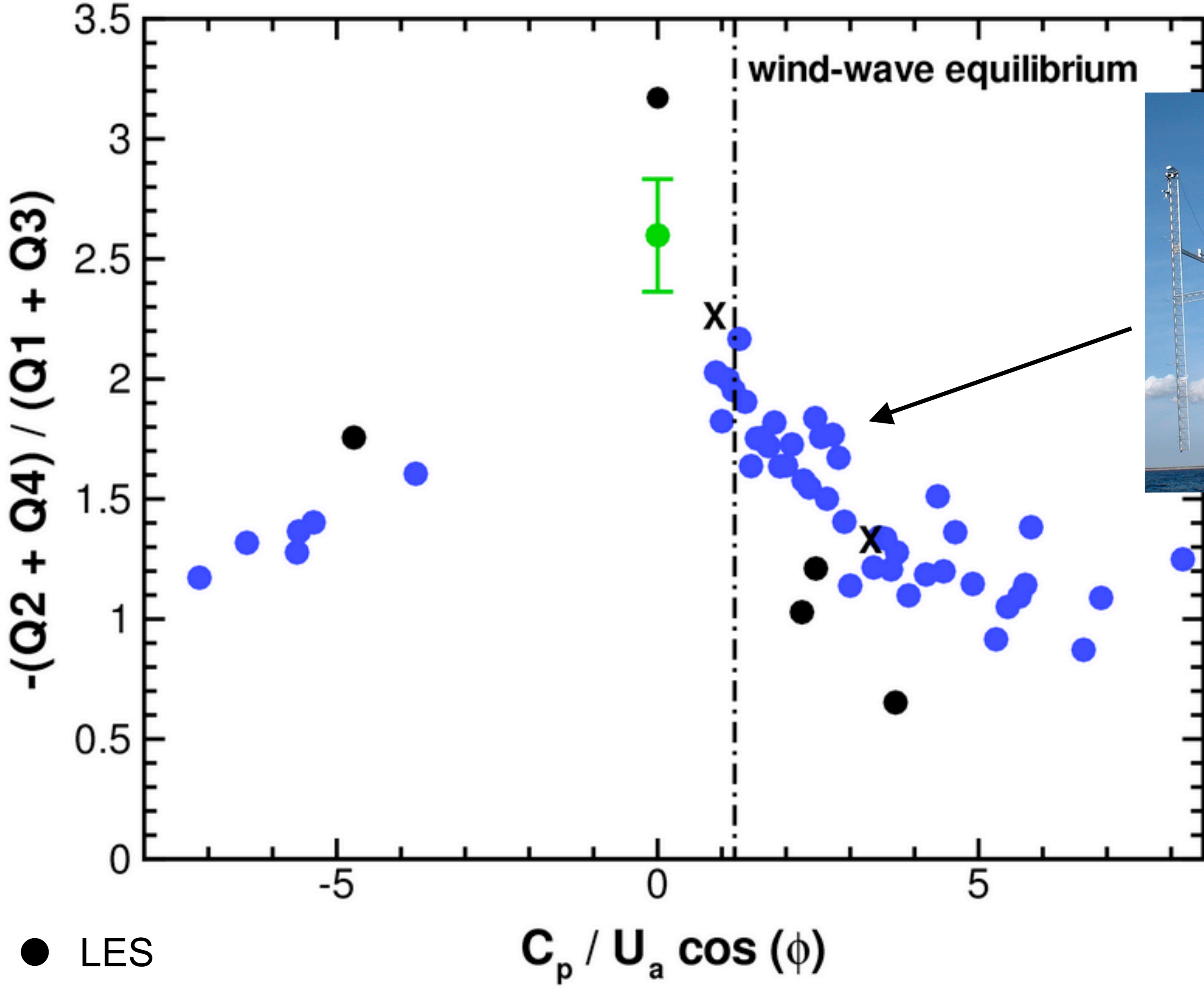
QUADRANT ANALYSIS OF $U'W'$ FROM CBLAST-LOW



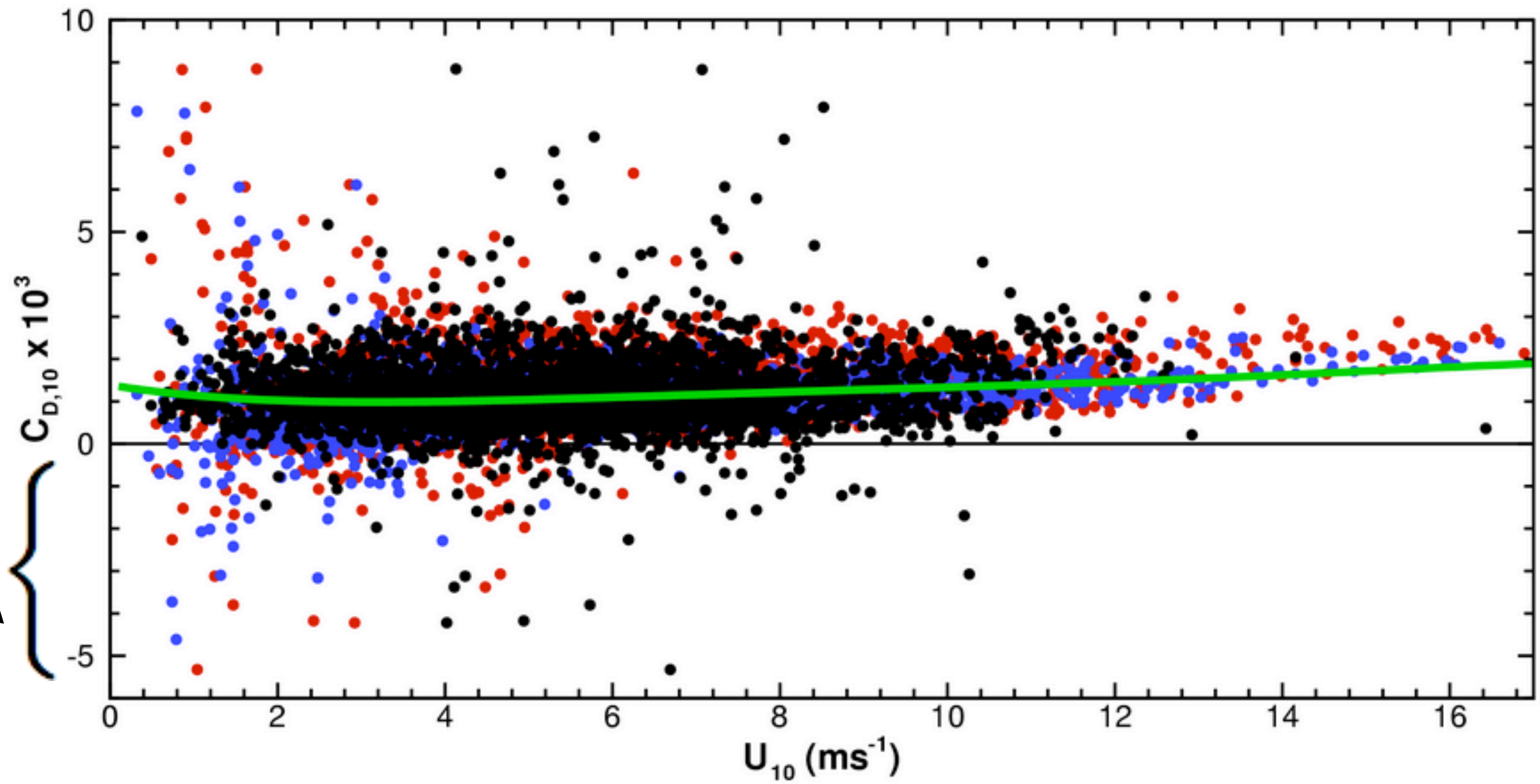
QUADRANT ANALYSIS OF $U'W'$ FROM CBLAST-LOW



QUADRANT ANALYSIS OF $U'W'$ FROM CBLAST-LOW



NEUTRAL DRAG COEFFICIENT $C_{D,10}$ FROM CBLAST LOW



Wave-driven winds

TOGA-COARE parameterization

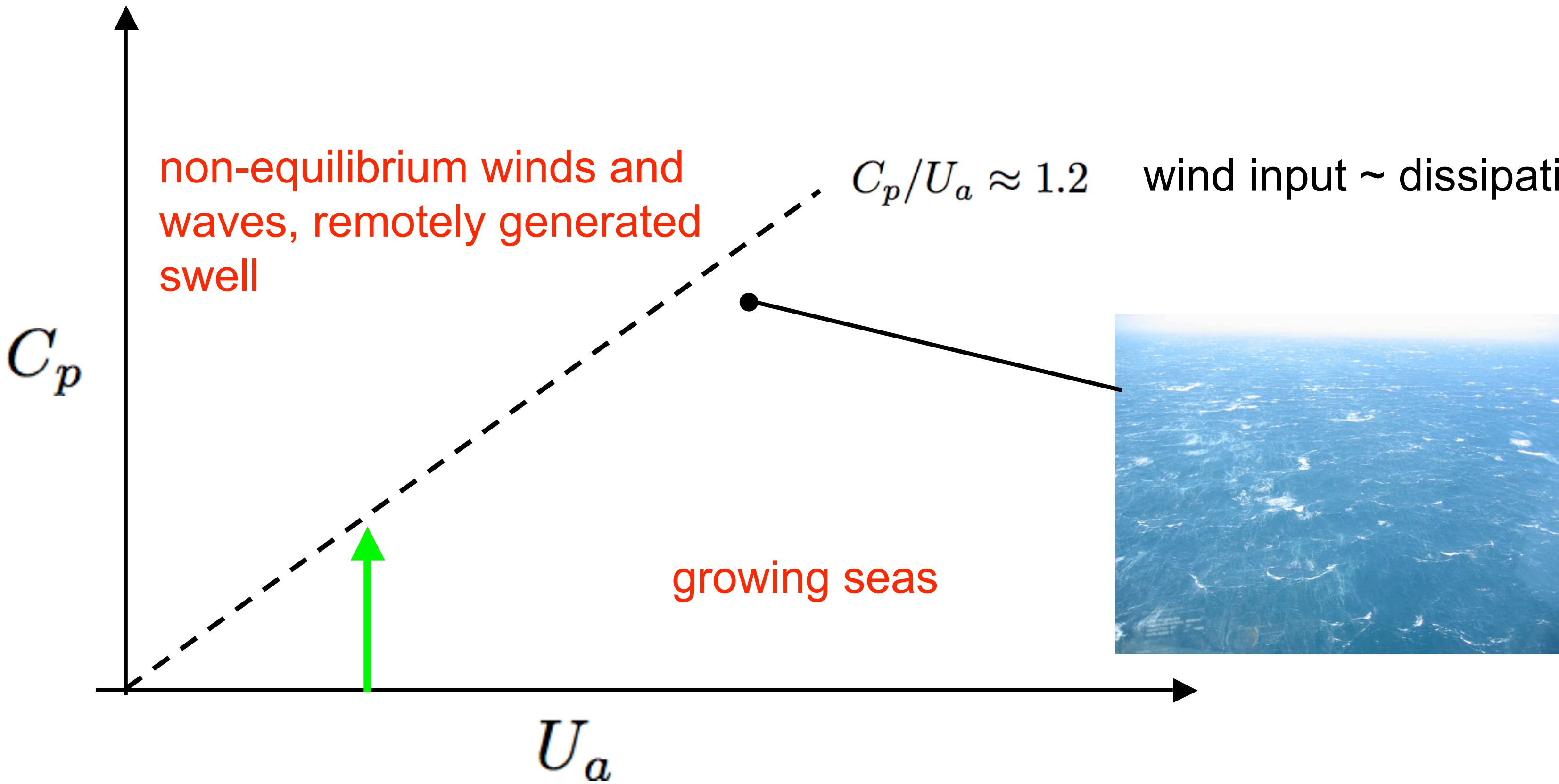
References

[*Sullivan et al.*(2008)] Sullivan, P. P., J. B. Edson, T. Hristov, and J. C. McWilliams. Large eddy simulations and observations of atmospheric marine boundary layers above non-equilibrium surface waves. *J. Atmos. Sci.*, 65:1225–1245, 2008.

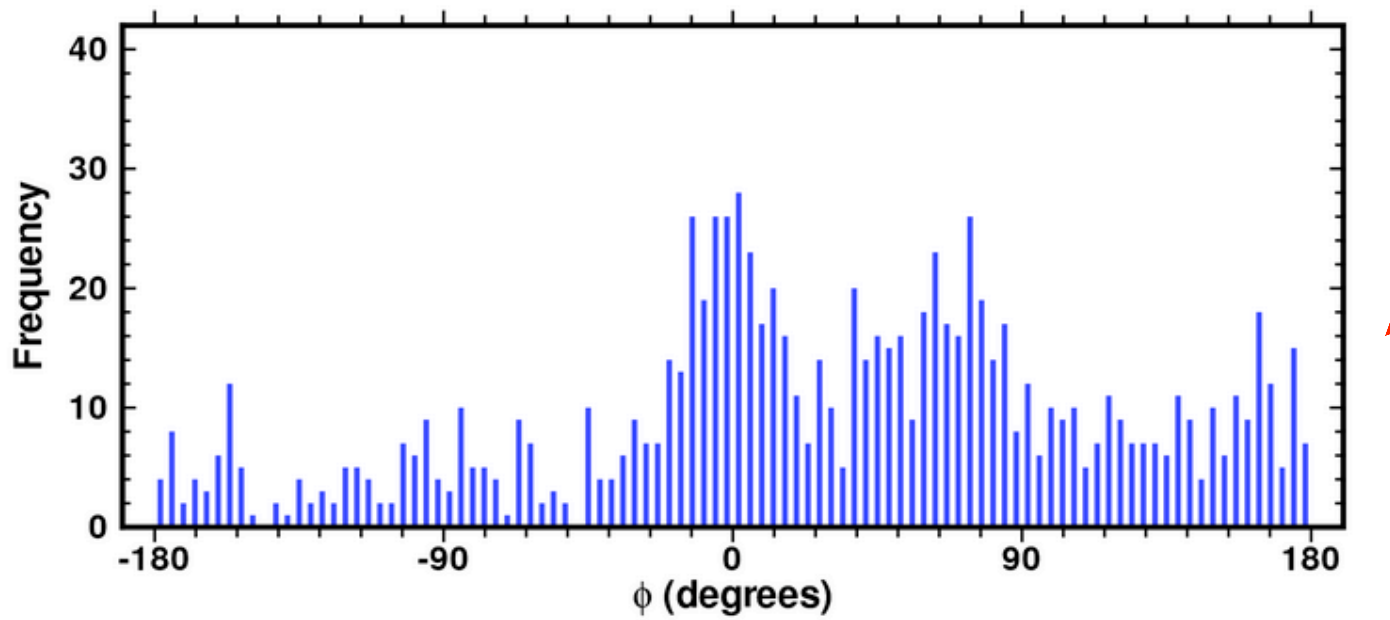
[*Sullivan et al.*(2007)] Sullivan, P. P., J. C. McWilliams, and W. K. Melville. Surface gravity wave effects in the oceanic boundary layer: Large-eddy simulation with vortex force and stochastic breakers. *J. Fluid Mech.*, 593:405–452, 2007.

[*Sullivan and Patton*(2008)] Sullivan, P. P. and E. G. Patton. A highly parallel algorithm for turbulence simulations in planetary boundary layers: Results with meshes up to 1024^3. In *18th Amer. Meteorol. Soc. Symp. on Boundary Layer and Turbulence*. Stockholm, Sweden, 2008.

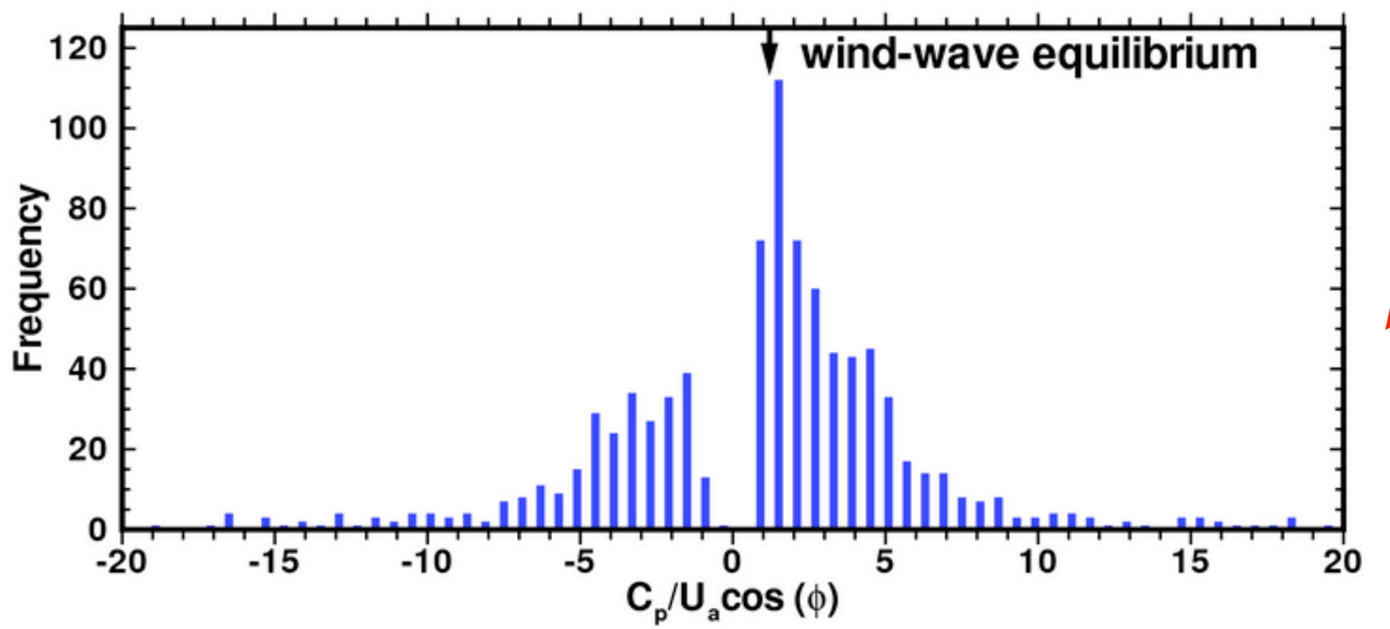
WAVE AGE, WIND-WAVE ALIGNMENT DEFINITIONS



NON-EQUILIBRIUM WINDS AND WAVES (CBLAST)



Wind-wave angle



Wave age