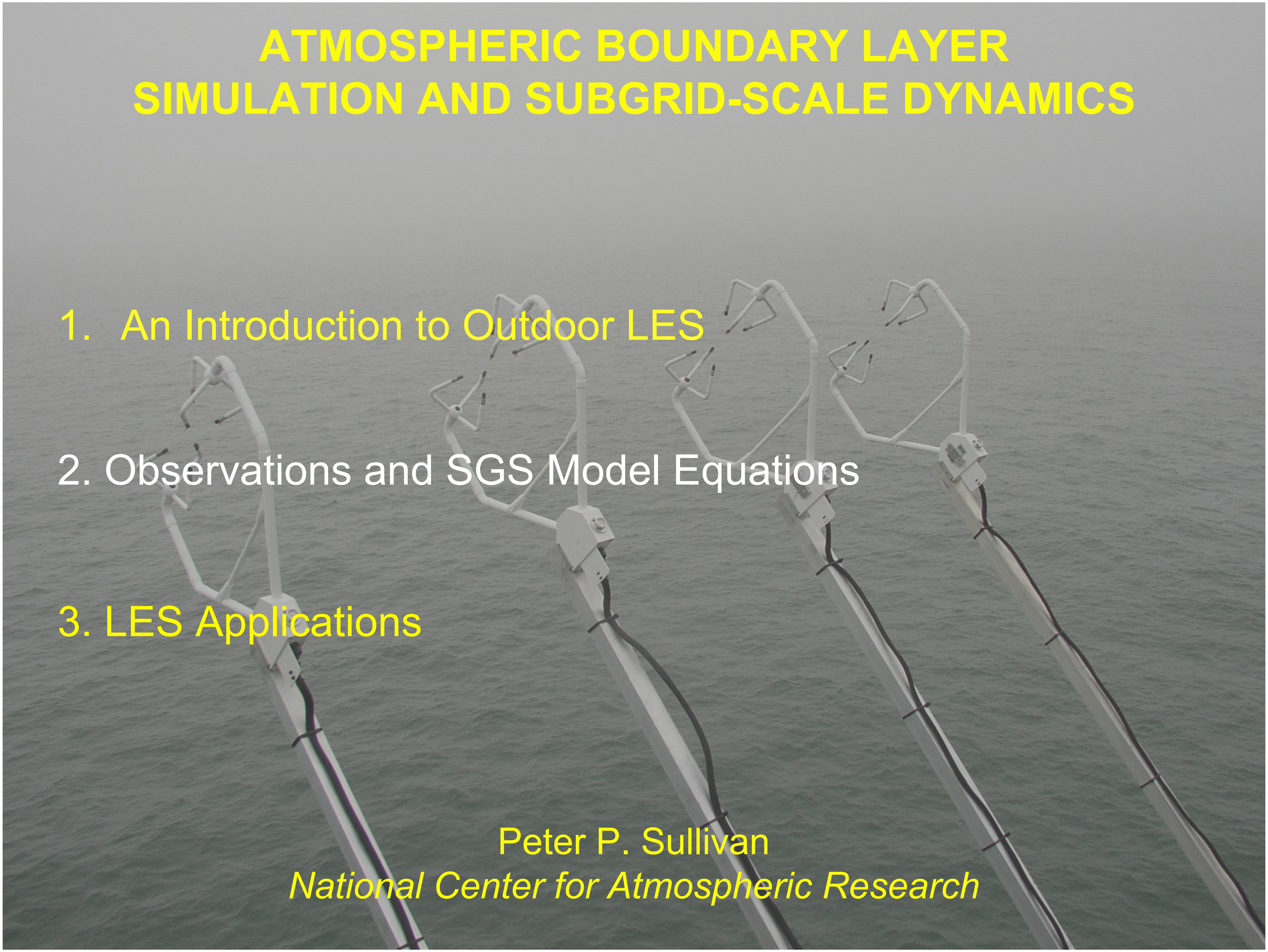


ATMOSPHERIC BOUNDARY LAYER SIMULATION AND SUBGRID-SCALE DYNAMICS

1. An Introduction to Outdoor LES

2. Observations and SGS Model Equations

3. LES Applications

Peter P. Sullivan
National Center for Atmospheric Research

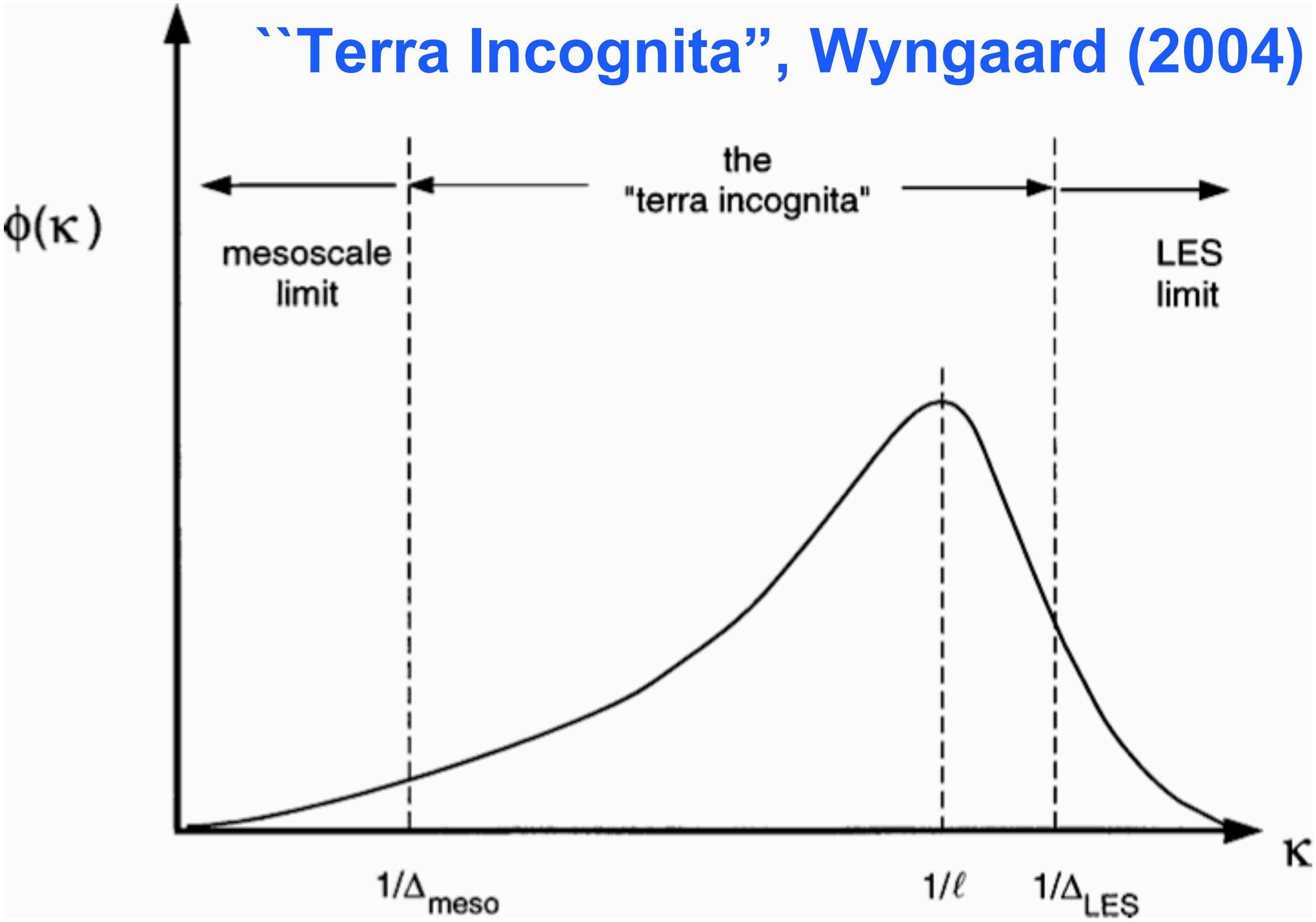


FIG. 1. A schematic of the turbulence spectrum $\phi(\kappa)$ in the horizontal plane as a function of the horizontal wavenumber magnitude κ. Its peak is at $\kappa \sim 1/l$, with l the length scale of the energetic eddies; Δ is the scale of the smoothing filter. In the mesoscale limit (left), $\Delta_{meso} \gg l$ and none of the turbulence is resolved. In the LES limit (right), $\Delta_{LES} \ll l$ and the energy-containing turbulence is resolved.

Where is your ``LES" ?

LARGE-EDDY SIMULATIONS AND OBSERVATIONS

Why LES of the PBL:

- Outdoor 4-D measurements are challenging
- Unsteady nature of the atmosphere and ocean
- Systematic investigation of the parameter space
- *Advances in parallel computing*

Gulf of Tehuantepec U ~[20-25] m/s

Validating/Improving LES with observations:

- Test the output
- Test the input subgrid-scale parameterizations

APPROACHES TO SUBGRID SCALE MODELING

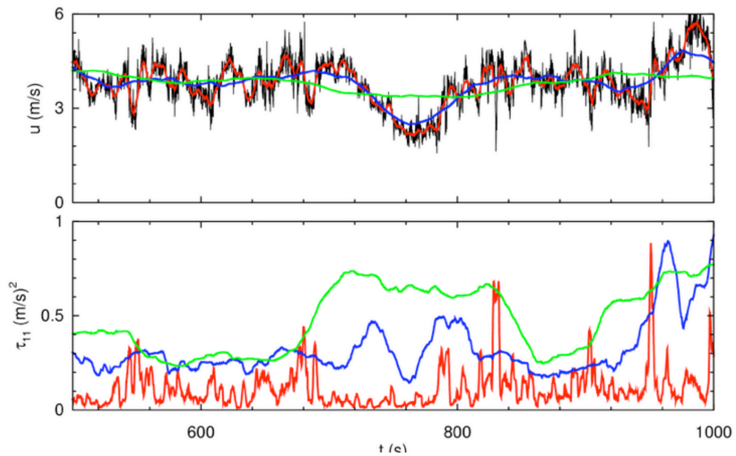
SGS parameterizations are physical models for small scale processes and filters that stabilize the numerical scheme.

- Traditional approaches to building SGS models
  - Lean on theory, $e.g.$, analysis by Lilly and others
  - Filter DNS databases to obtain resolved and SGS pieces

- The literature is vast, especially in physics/engineering
  - Simple algebraic models $e.g.$, Smagorinsky
  - Stochastic approaches [*Mason and Thomson*(1992)]
  - One equation TKE models [*Deardorff*(1980)]
  - Hybrid TKE/RANS [*Sullivan et al.*(1994)]
  - Algebraic Reynolds stress models [*Schmidt and Schumann*(1989)]
  - Dynamic models [*Germano et al.*(1991)]
  - Nonlinear mixed models [*Meneveau and Katz*(2000)]
  - Deconvolution methods [*Stolz et al.*(2001)]
  - Velocity estimation models [*Dubrulle et al.*(2002)]
  - Algorithmic models [*Domaradzki and Horiuti*(2001)]
  - Transport equations [*Wyngaard*(2004)]

Can we use targeted observations to provide insight as to the nature of SGS motions in high Re PBLs?

HIGH REYNOLDS NUMBER OBSERVATIONS AND LES

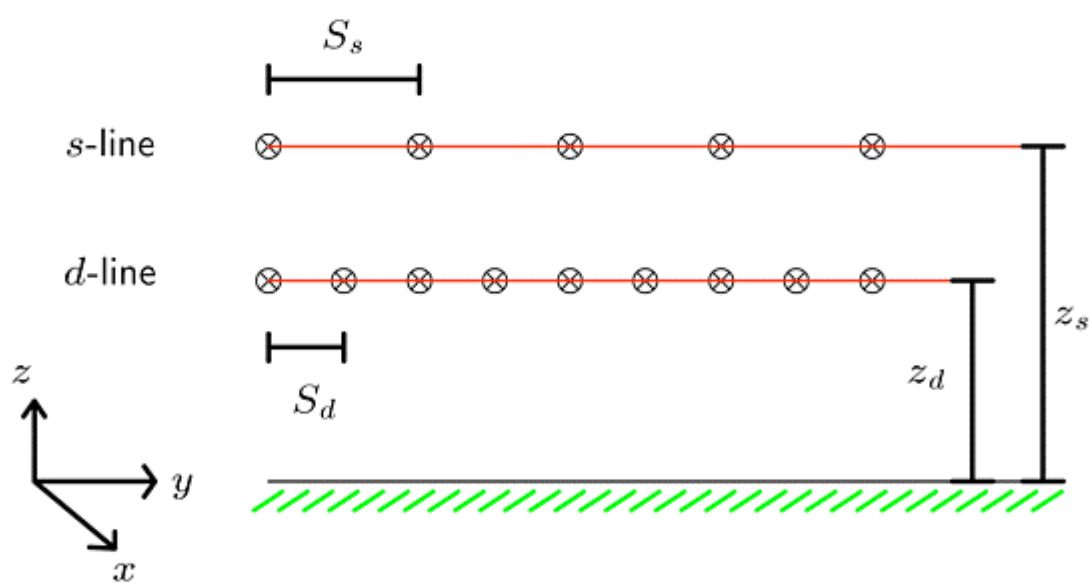


- **SINGLE-POINT MEASUREMENTS**
  - Cannot be used directly to improve LES

- **MULTI-POINT MEASUREMENTS**
  - Span a range of filter widths, $e.g.$, $\mathcal{O}$(m) to $\mathcal{O}$(100m)
  - Ideally 3-D, time varying "volume" of turbulence and scalars in canonical flows with shear, stratification, near boundaries, ...
  - Horizontal Array Turbulence Study field campaigns, HATS (2000), OHATS (2004), CHATS (2007), AHATS (2008)

HORIZONTAL ARRAY TURBULENCE STUDY (HATS)

- Field campaign to measure $\mathcal{T}_{ij}, \mathcal{T}_{i\theta}$ over a wide range of stratification Horst *et al.* (2002)
- Based on the horizontal array technique Tong *et al.* (1998), (1999) and Porté-Agel *et al.* (2001)
- 4 different sonic arrays, $-2 < z/L < 2$



RATIONALE FOR EXPERIMENTAL DESIGN

- Allows *spatial* filtering of flow field and decomposition into resolved and subfilter scale velocities $(\overline{U_i}, u_i)$:

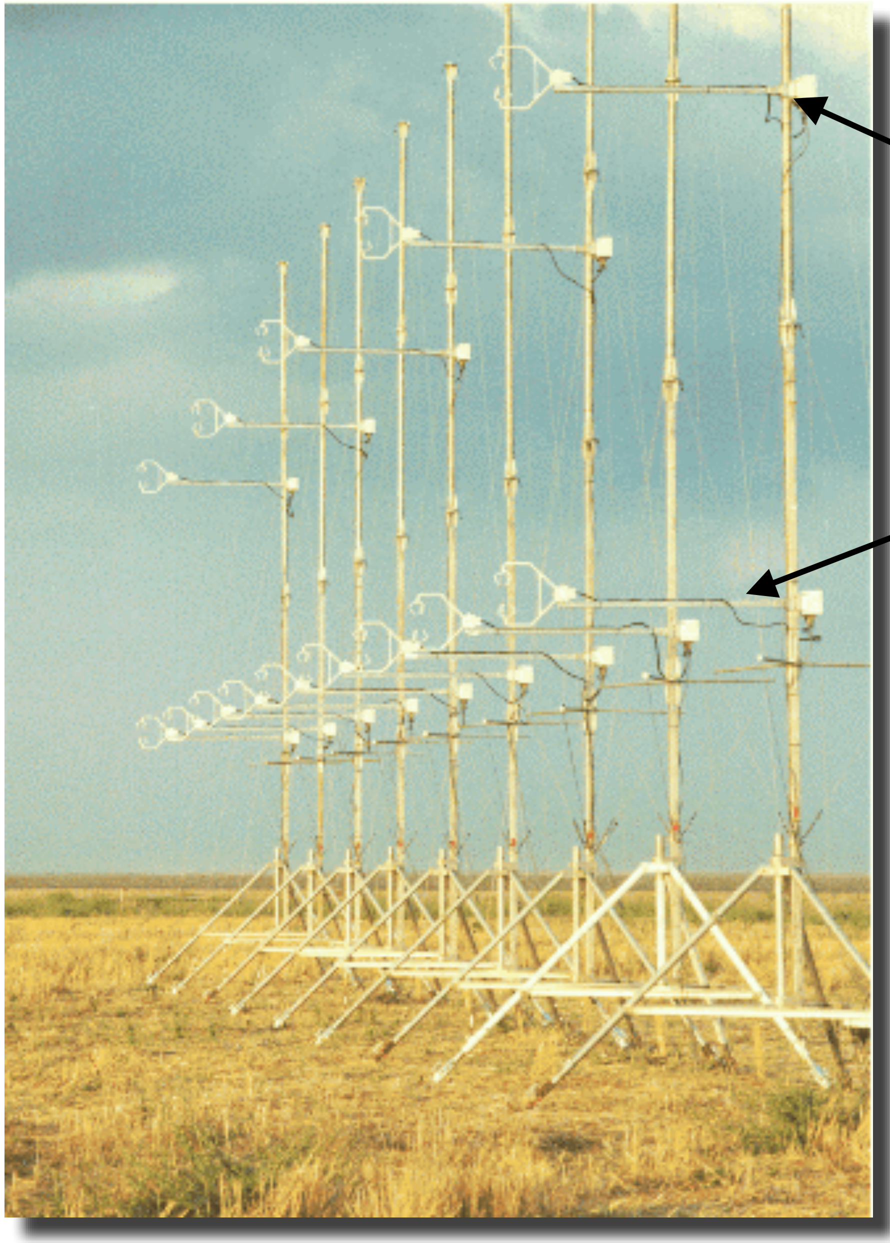
$$U_i = \overline{U_i} + u_i \equiv \int U(x'_j)G(x_i, x'_j)dx'_j + u_i$$

- Allows construction of SFS fluxes:

$$\mathcal{T}_{ij} = \overline{U_i U_j} - \overline{U_i}\,\overline{U_j}$$

- Allows measurement of resolved gradients $\partial\overline{U_i}/\partial x$, $\partial\overline{U_i}/\partial y$ and $\partial\overline{U_i}/\partial z$

- Allows expansion of SFS fluxes $\mathcal{T}_{ij}$ into Leonard, Cross, and Reynolds terms which requires *double* spatial filtering, *e.g.*, $\overline{\overline{U_i} u_j}$



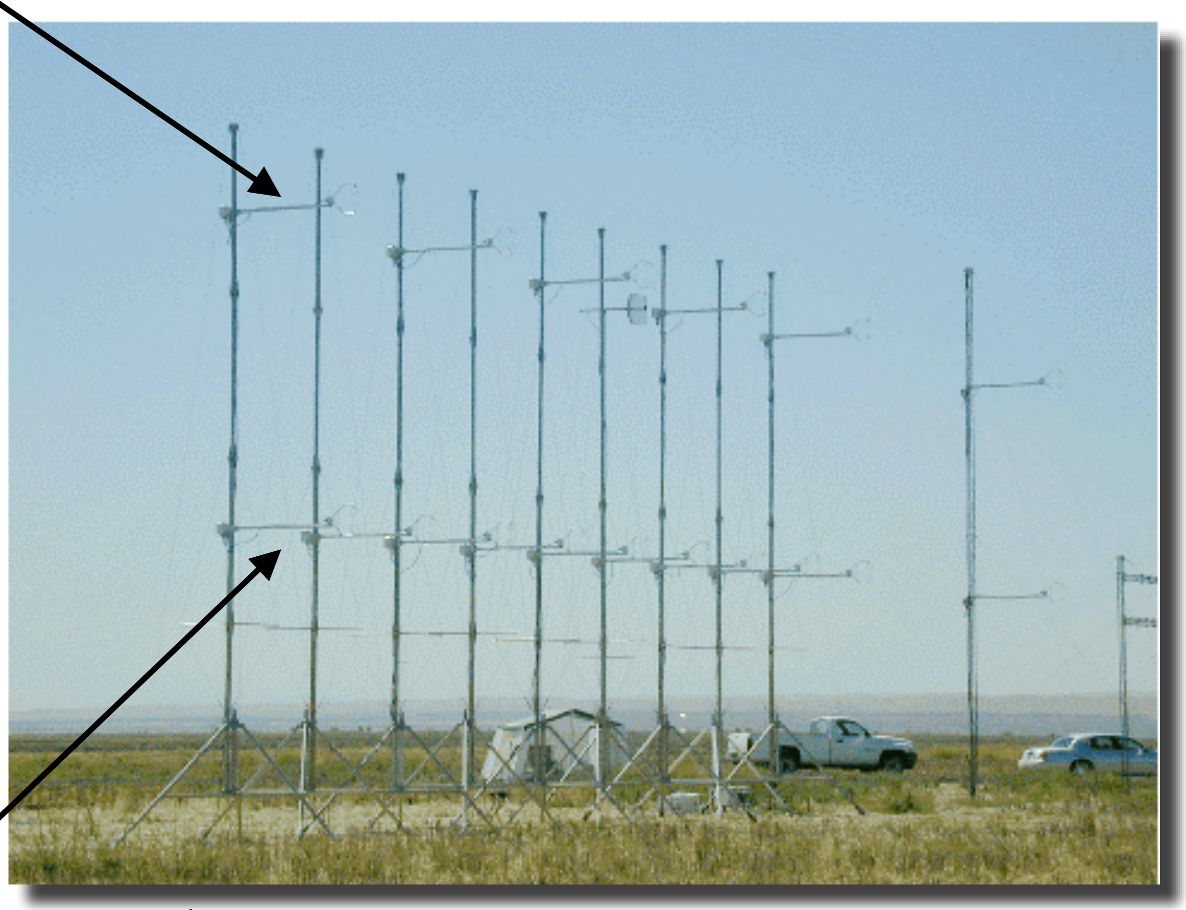
$z_s = 6.90\text{m}, dy_s = 6.70\text{m}$

$z_d = 3.45\text{m}, dy_d = 3.35\text{m}$

ARRAY-1

ARRAY-2

$z_s = 8.66$m, $dy_s = 4.33$m



$z_d = 4.33$m, $dy_d = 2.17$m

ARRAY-3

$z_d = 8.66\text{m},\ dy_d = 2.17\text{m}$

$z_s = 4.33\text{m},\ dy_s = 1.08\text{m}$

ARRAY-4

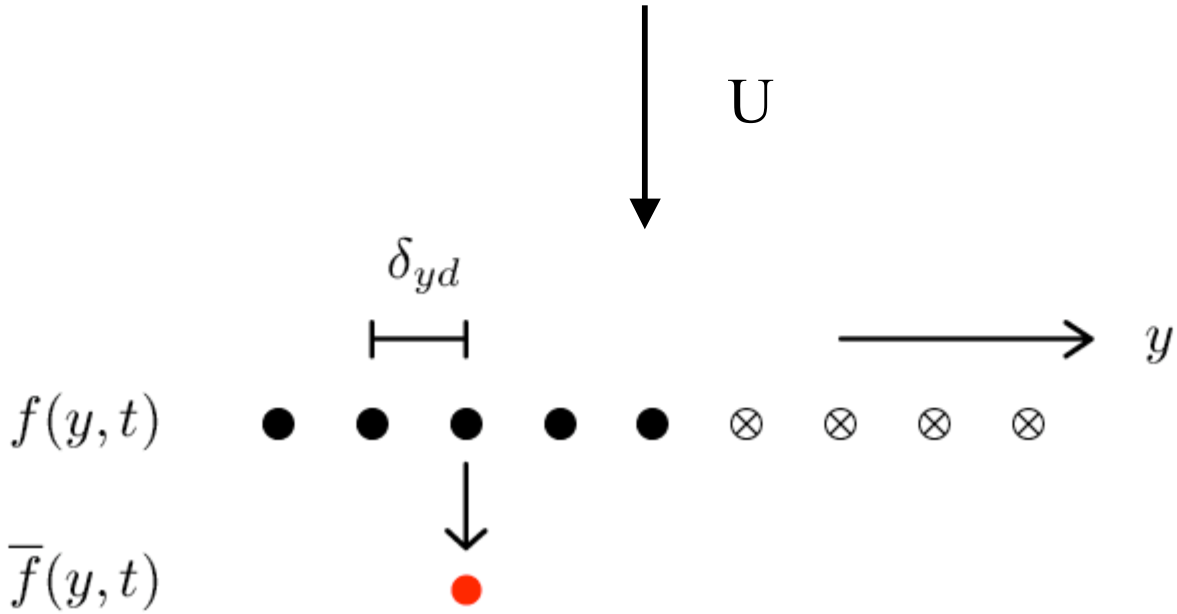
$z_s = 5.15$m

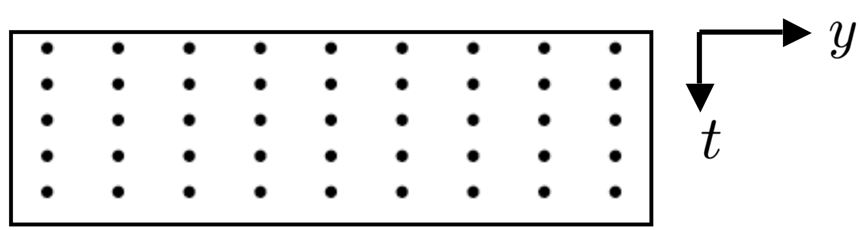
$dy_s = 0.63$m

$z_d = 4.15$m

$dy_d = 0.50$m

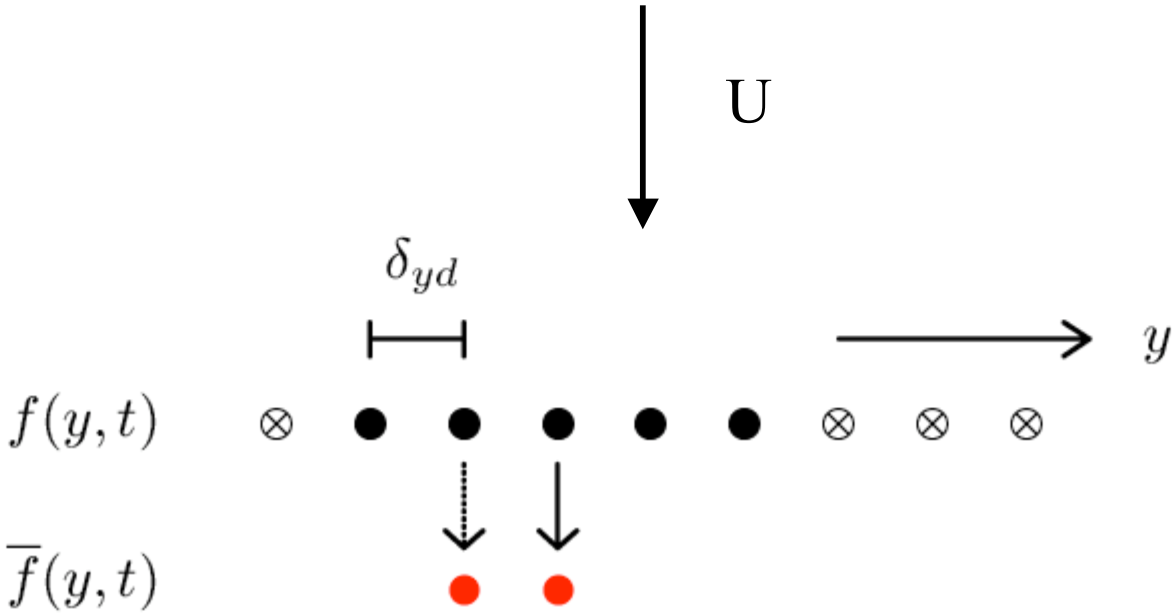
AN EXAMPLE OF LATERAL (Y) FILTERING



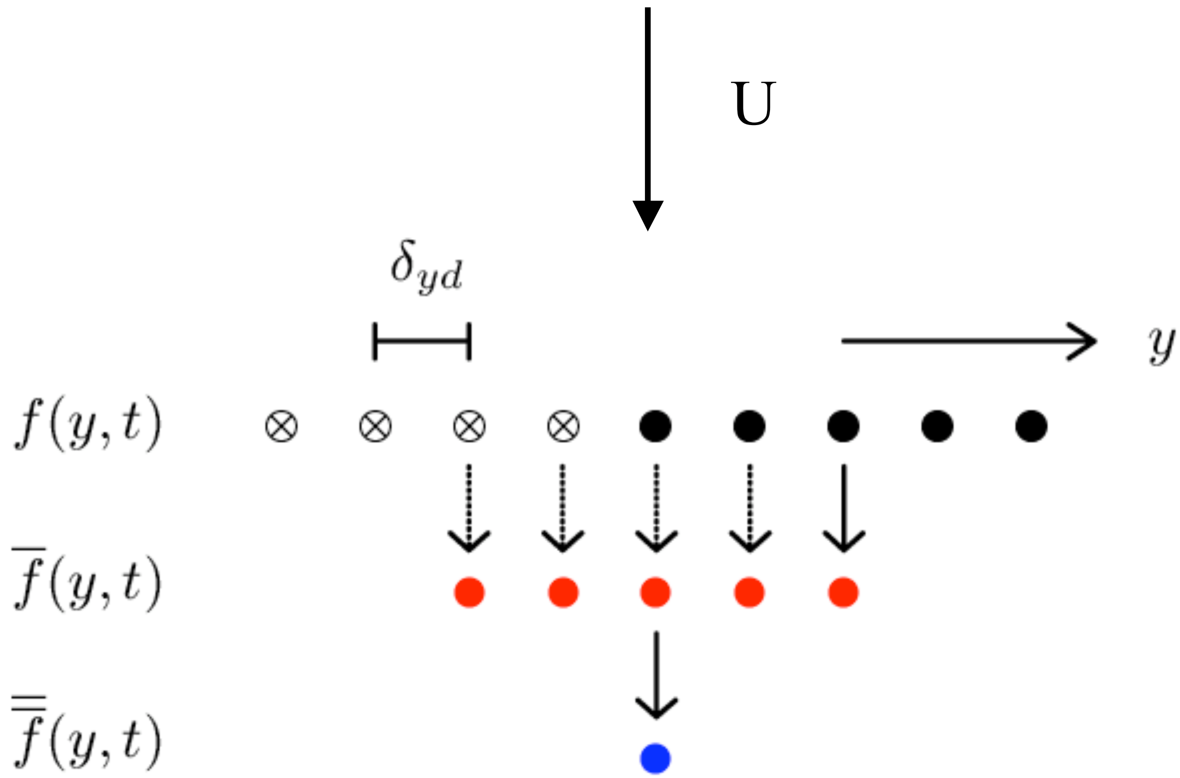


``2D plane of turbulence”

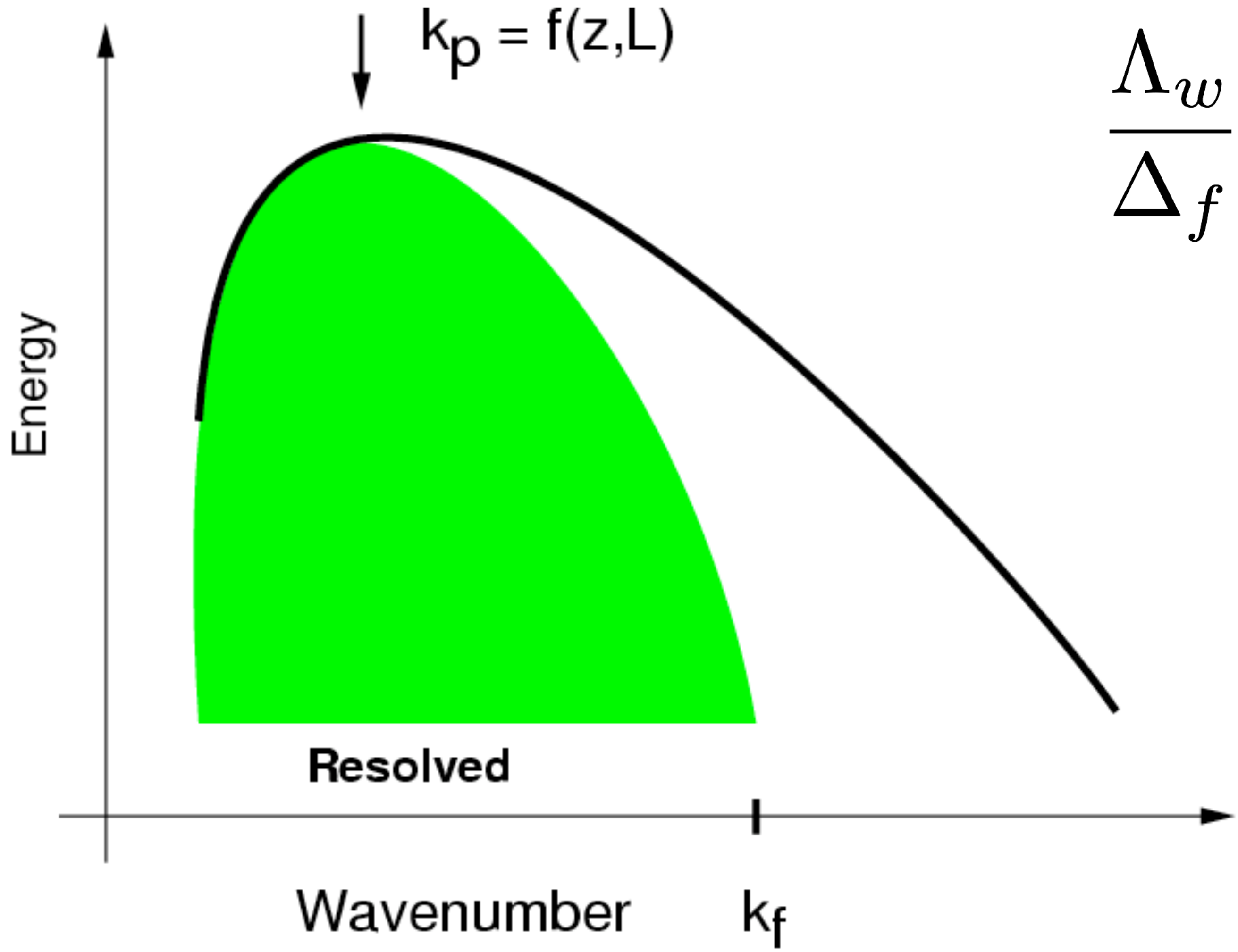
AN EXAMPLE OF LATERAL (Y) FILTERING



AN EXAMPLE OF LATERAL (Y) FILTERING

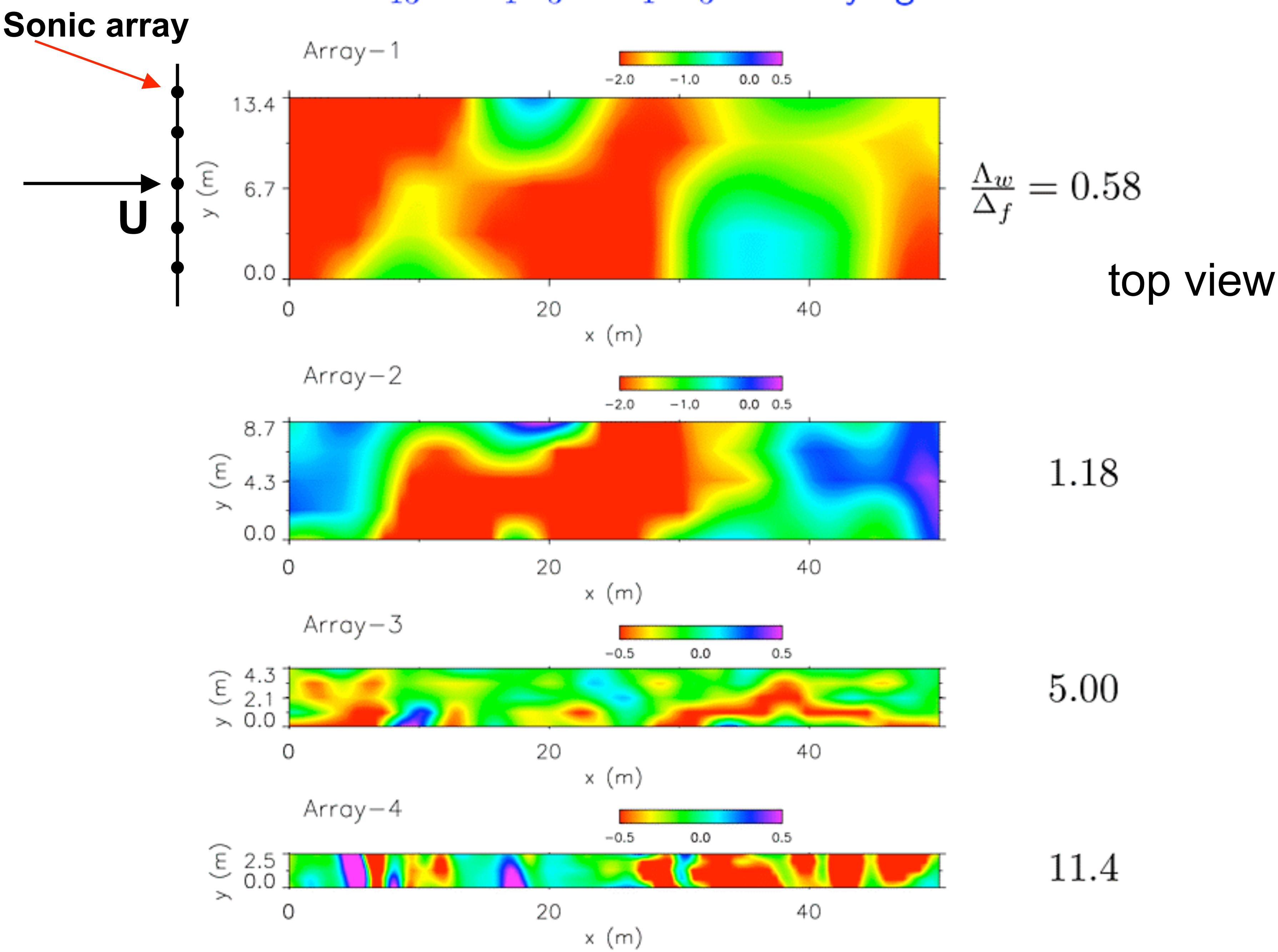


SPECTRAL PEAK AND FILTER CUTOFF WAVENUMBERS

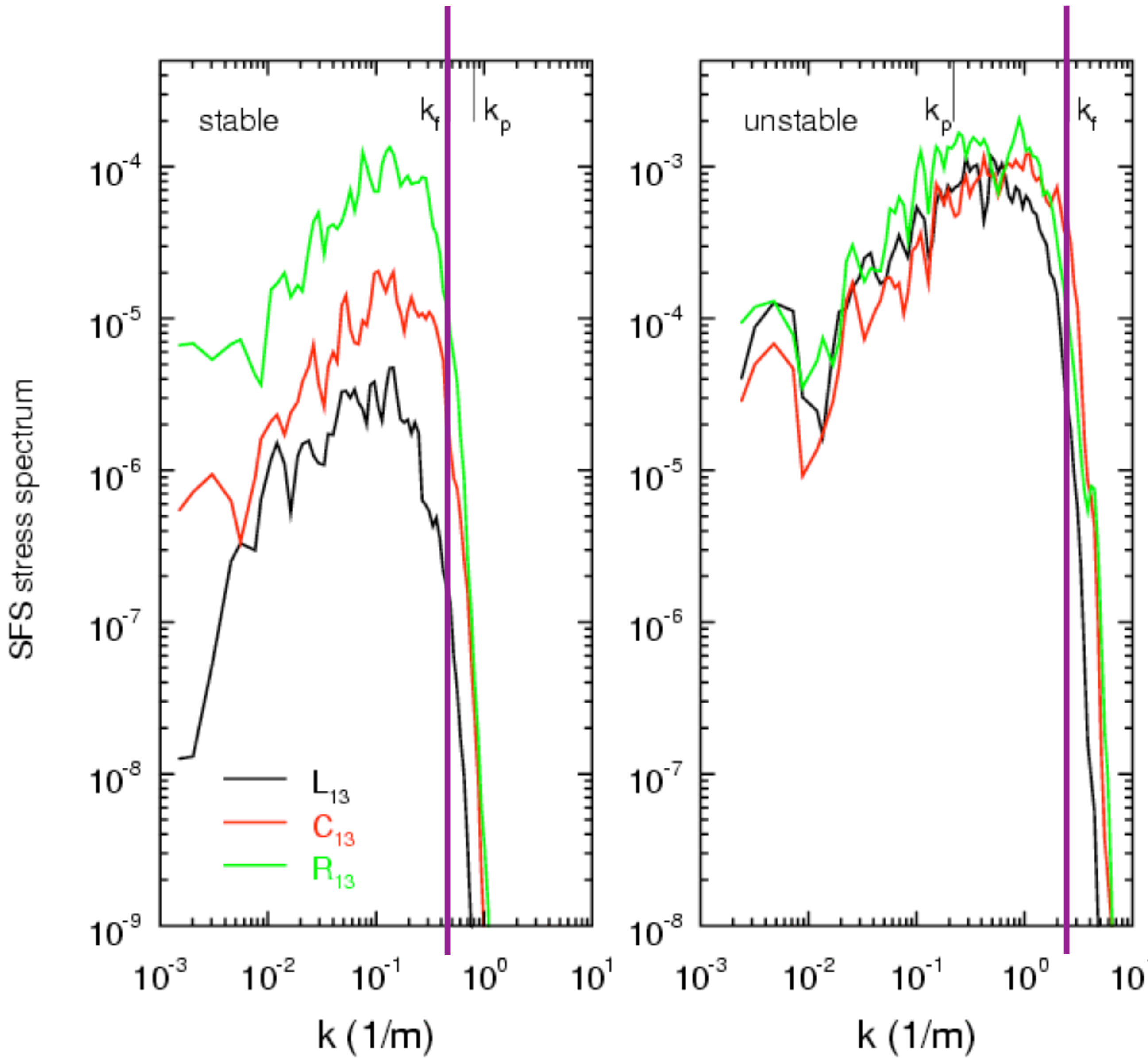


$$\frac{\Lambda_w}{\Delta_f}$$

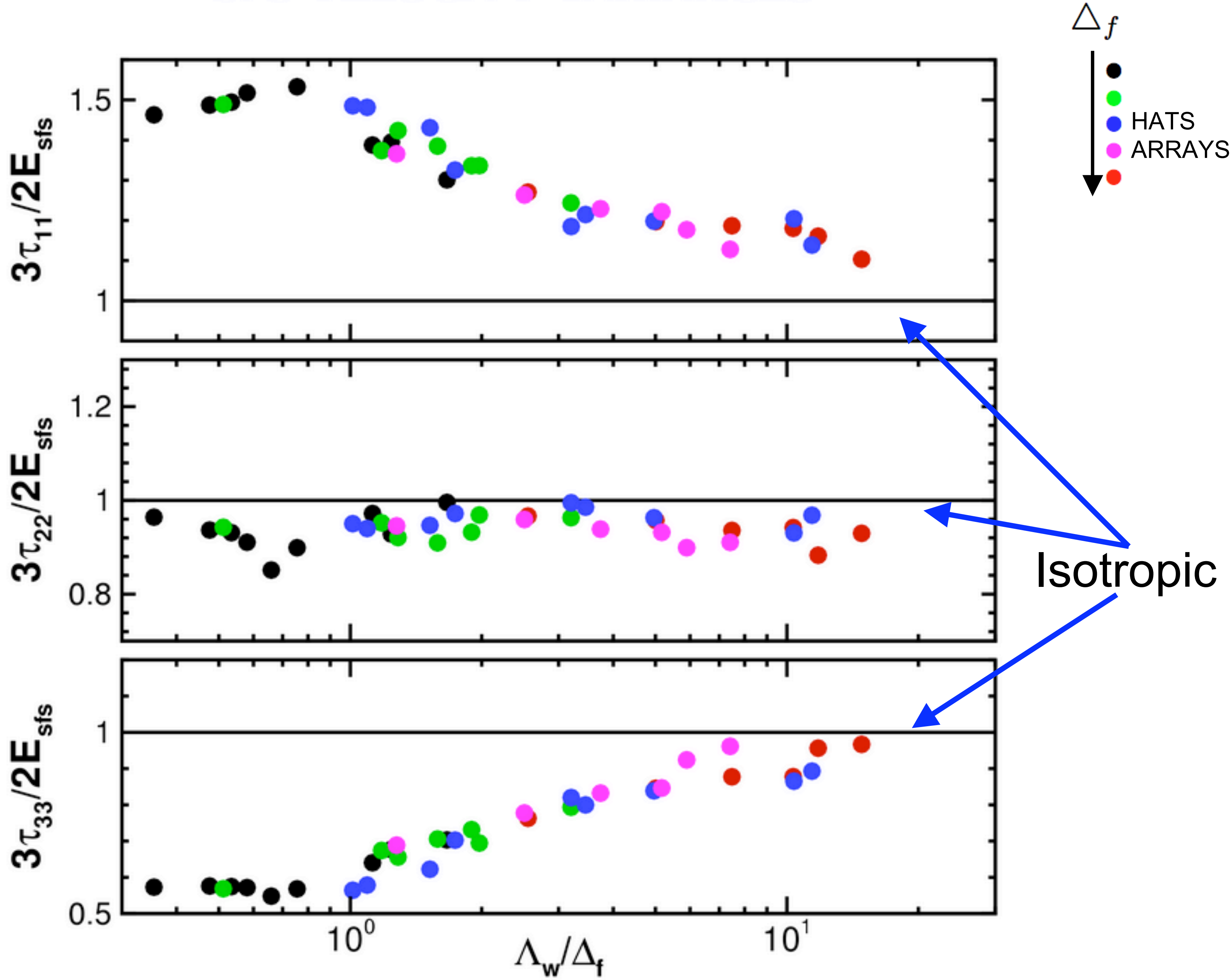
SFS Flux $\tau_{13} = \overline{U_1 U_3} - \overline{U_1}\ \overline{U_3}$ for Varying Filter Widths



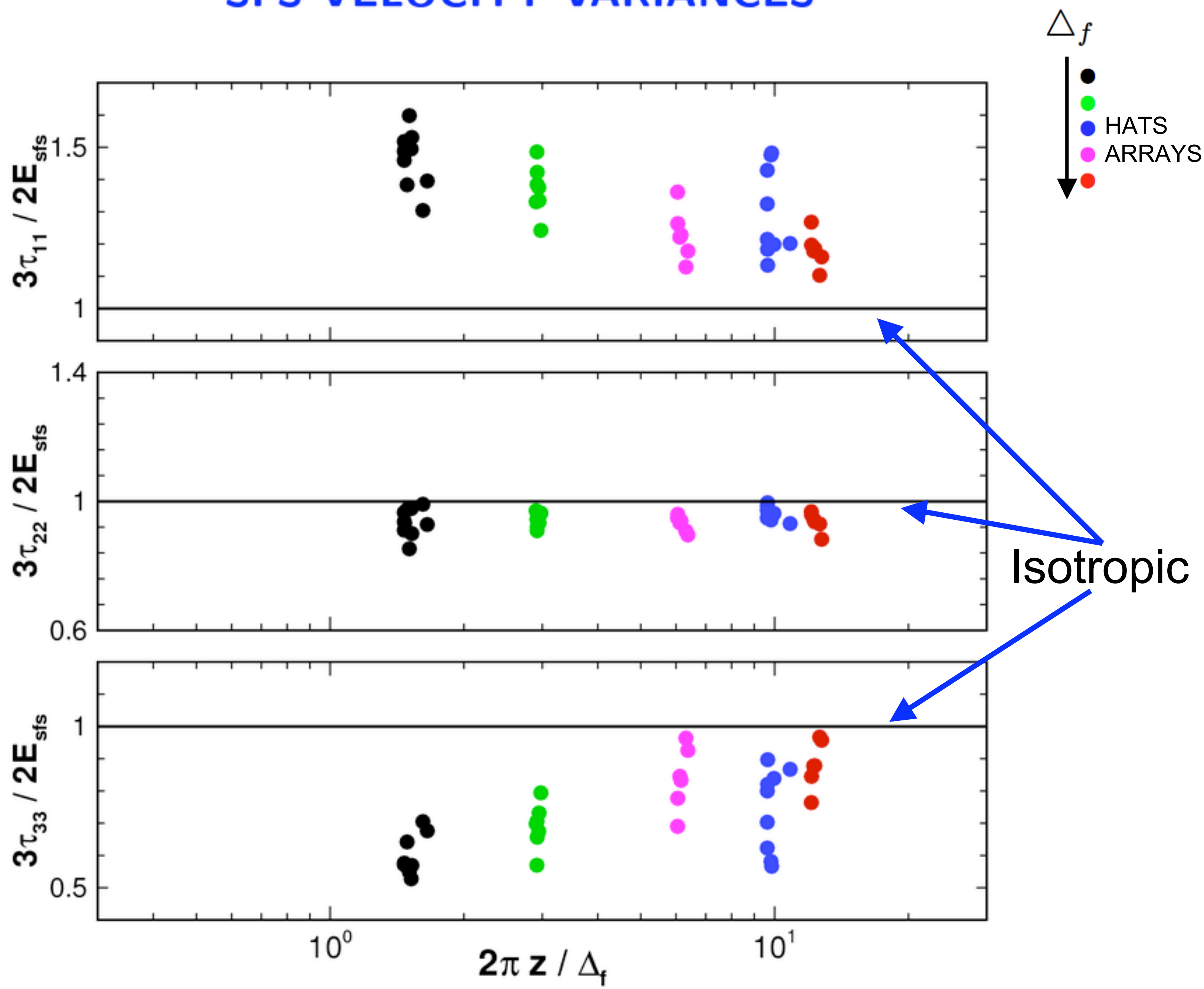
Spectra of Leonard, Cross, Reynolds Terms for (1,3) Component



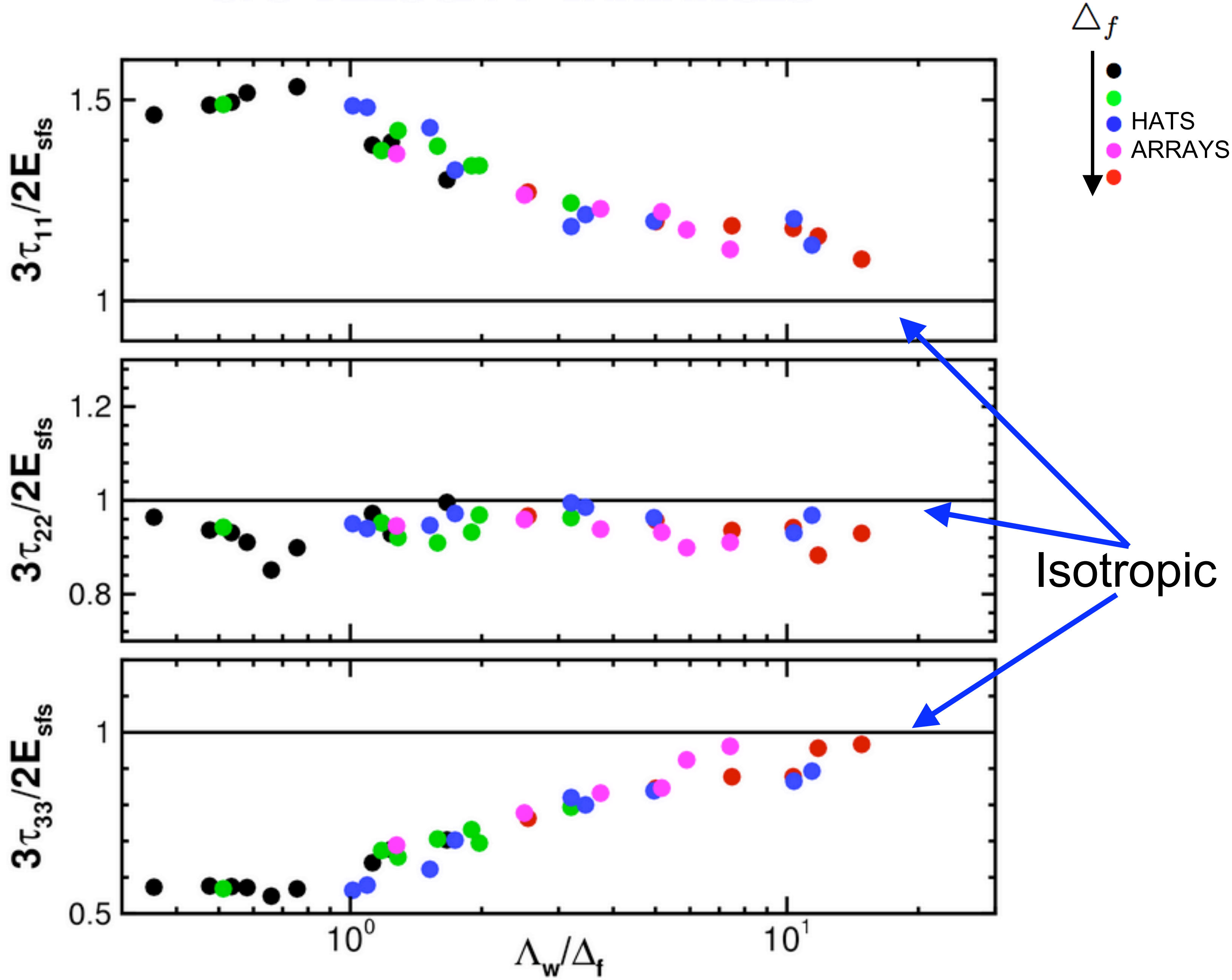
SFS VELOCITY VARIANCES



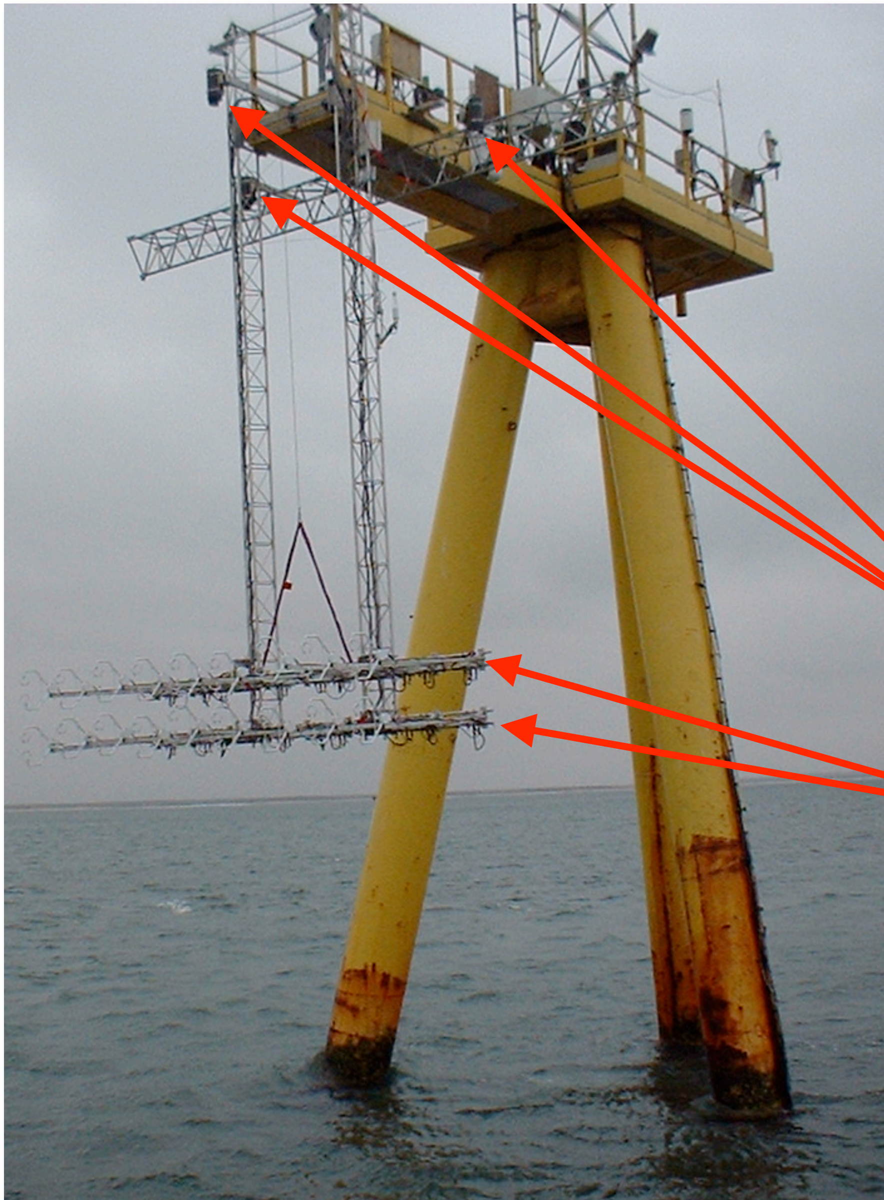
SFS VELOCITY VARIANCES

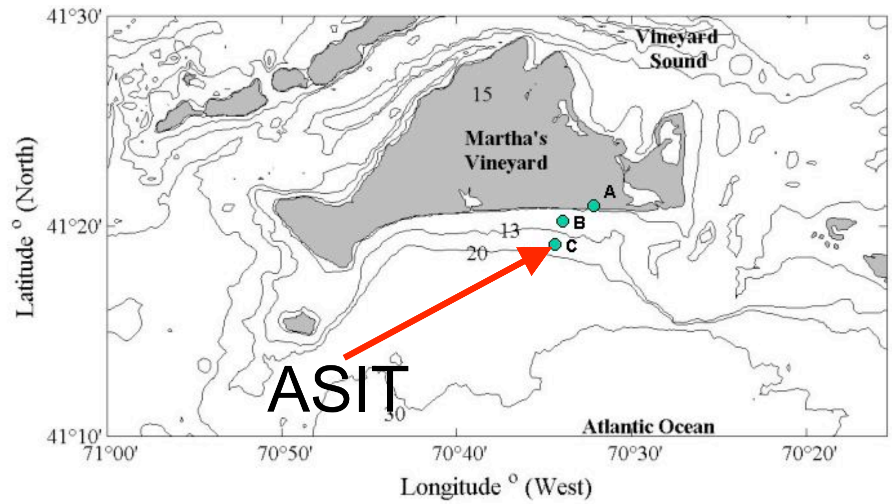


SFS VELOCITY VARIANCES



OHATS FIELD CAMPAIGN



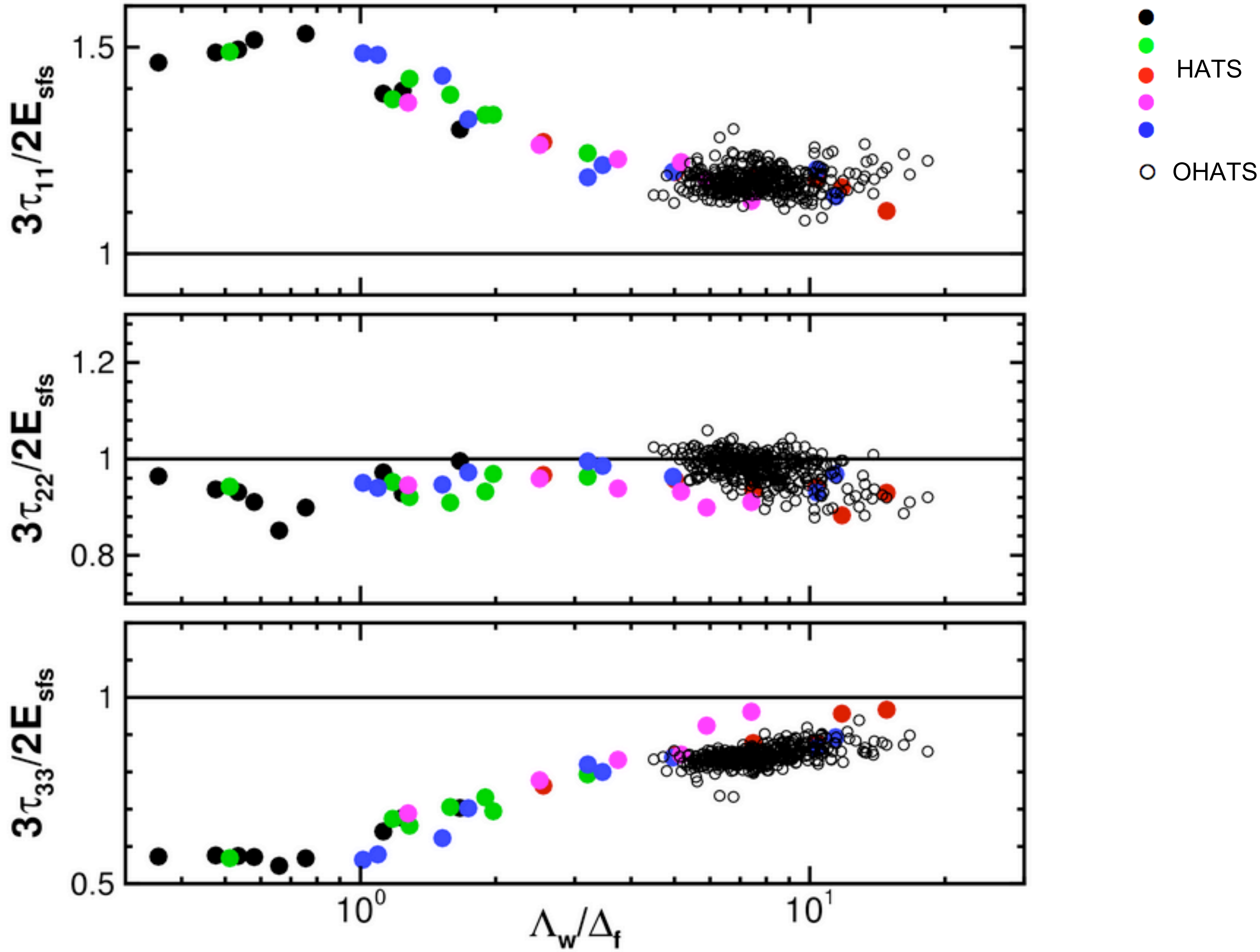


Laser altimeters

18 CSATS

275 hours ``12 days of data” analyzed

SFS VELOCITY VARIANCES



RATE EQUATIONS FOR SUBGRID DEVIATORIC STRESS

- What are the parent equations for the Smagorinsky model?

RATE EQUATIONS FOR SUBGRID DEVIATORIC STRESS

The SGS stress is

$$\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j$$

To get the "rate equation" for SGS τ_{ij}

$$\frac{\partial \tau_{ij}}{\partial t} = \left[\overline{u_j \frac{\partial u_i}{\partial t}} - \overline{u_j} \frac{\partial \overline{u}_i}{\partial t} \right]$$

Substitution steps:

$$u_j \frac{\partial u_i}{\partial t} = u_j \mathcal{R}_i \qquad \overline{u}_j \frac{\partial \overline{u}_i}{\partial t} = \overline{u}_j \overline{\mathcal{R}}_i$$

The difference is now τ_{ij} is the deviatoric stress, *i.e.*, $-2/3e\delta_{ij}$

Considerable Algebra !

RATE EQUATIONS FOR SUBGRID DEVIATORIC STRESS

- **What are the parent equations for the Smagorinsky model?**
  - Lilly (1967), Deardorff (1973), Wyngaard (2004), Hatlee & Wyngaard (2007)

Isotropic production

$$\begin{aligned}
\frac{D\tau_{ij}}{Dt} &= \frac{2}{3}e\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) \\
&\quad - \left[\tau_{ik}\frac{\partial \overline{u}_j}{\partial x_k} + \tau_{jk}\frac{\partial \overline{u}_i}{\partial x_k} - \frac{1}{3}\delta_{ij}\tau_{kl}\left(\frac{\partial \overline{u}_k}{\partial x_l} + \frac{\partial \overline{u}_l}{\partial x_k}\right)\right] \\
&\quad - \frac{1}{\rho}\left[\overline{p\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)} - \overline{p}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right)\right] \\
&\quad + \text{transport} + \text{buoyancy production}
\end{aligned}$$

Pressure destruction

Anisotropic deviatoric production

RATE EQUATIONS FOR SUBGRID DEVIATORIC STRESS

- **What are the parent equations for the Smagorinsky model?**
  - Lilly (1967), Deardorff (1973), Wyngaard (2004), Hatlee & Wyngaard (2007)

$$
\begin{aligned}
\cancelto{0}{\frac{D\tau_{ij}}{Dt}} = \; & \frac{2}{3}e\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) \\
& - \cancelto{0}{\left[\tau_{ik}\frac{\partial \bar{u}_j}{\partial x_k} + \tau_{jk}\frac{\partial \bar{u}_i}{\partial x_k} - \frac{1}{3}\delta_{ij}\tau_{kl}\left(\frac{\partial \bar{u}_k}{\partial x_l} + \frac{\partial \bar{u}_l}{\partial x_k}\right)\right]} \\
& - \frac{1}{\rho}\left[\overline{p\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)} - \bar{p}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)\right] \\
& + \cancelto{0}{\text{transport}} + \cancelto{0}{\text{buoyancy production}}
\end{aligned}
$$

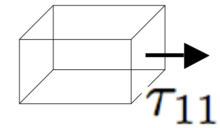
Rotta model

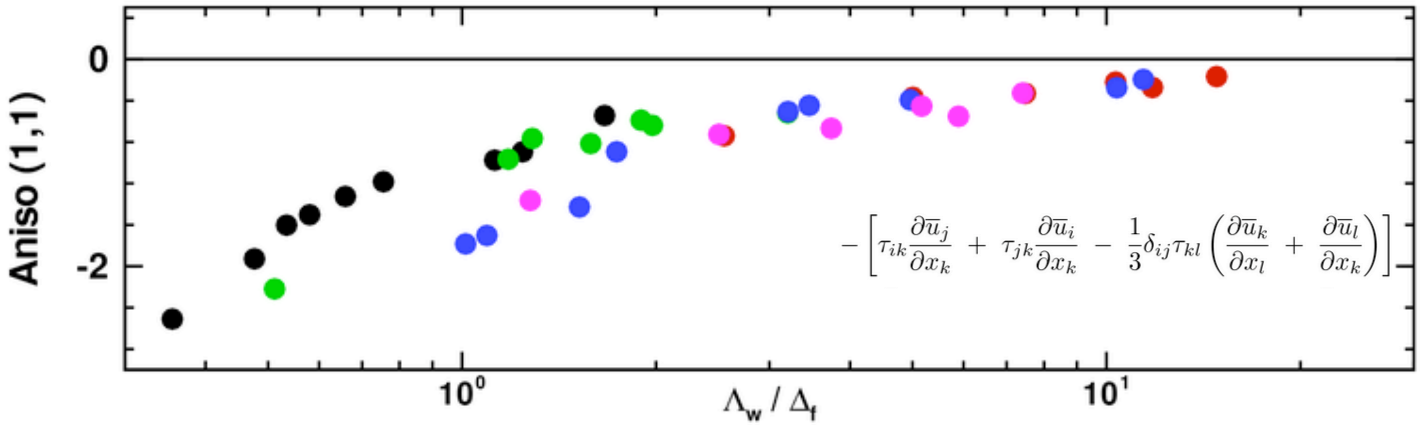
$$
\boxed{\frac{\tau_{ij}}{T} = \frac{2}{3}e\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)}
$$

Time scale

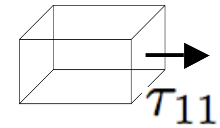
$$
T = c\,\frac{\Delta_f}{\sqrt{e}}
$$

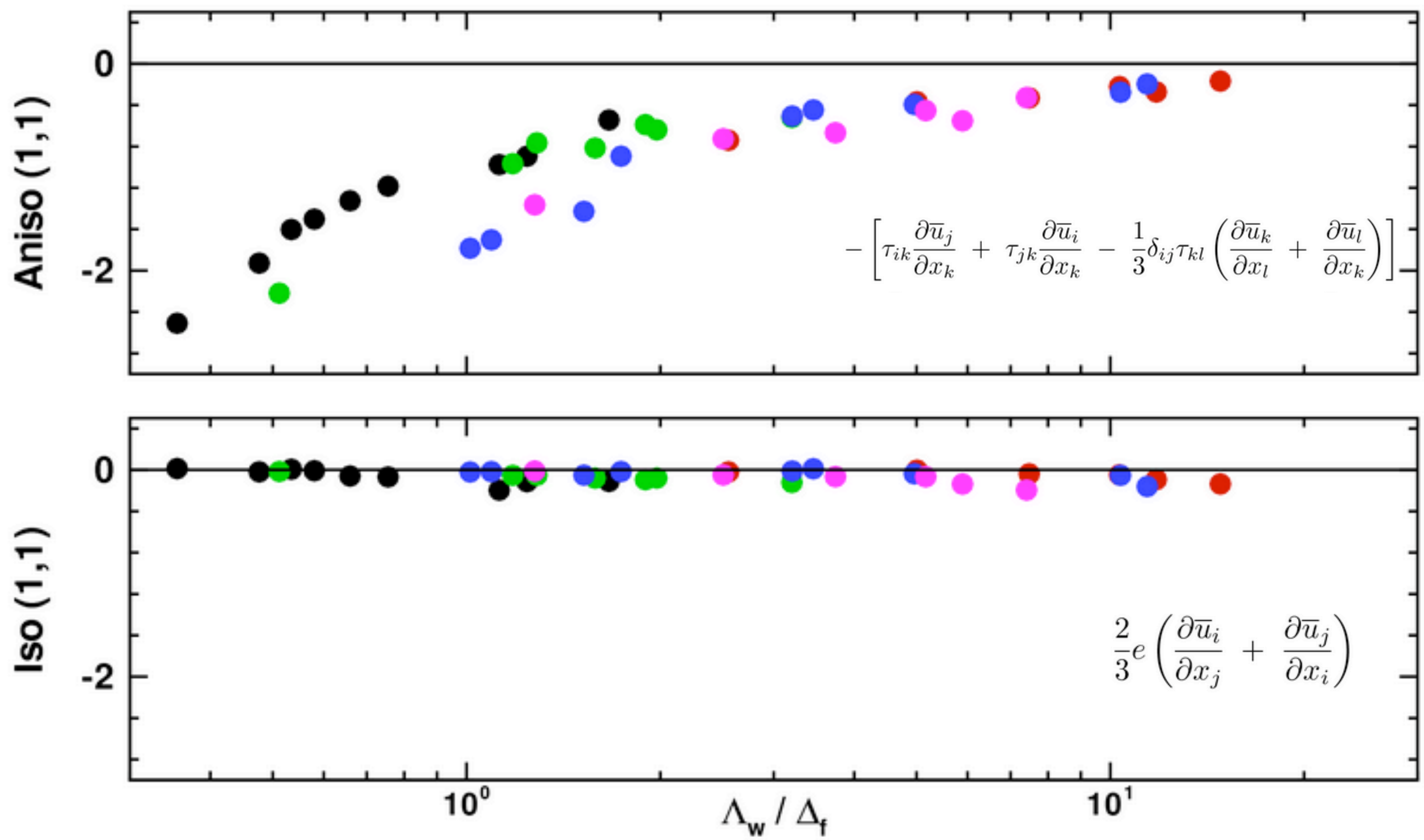
PRODUCTION OF SUBFILTER SCALE FLUX τ_{11}



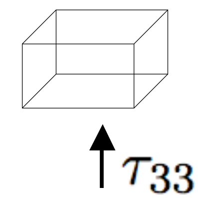


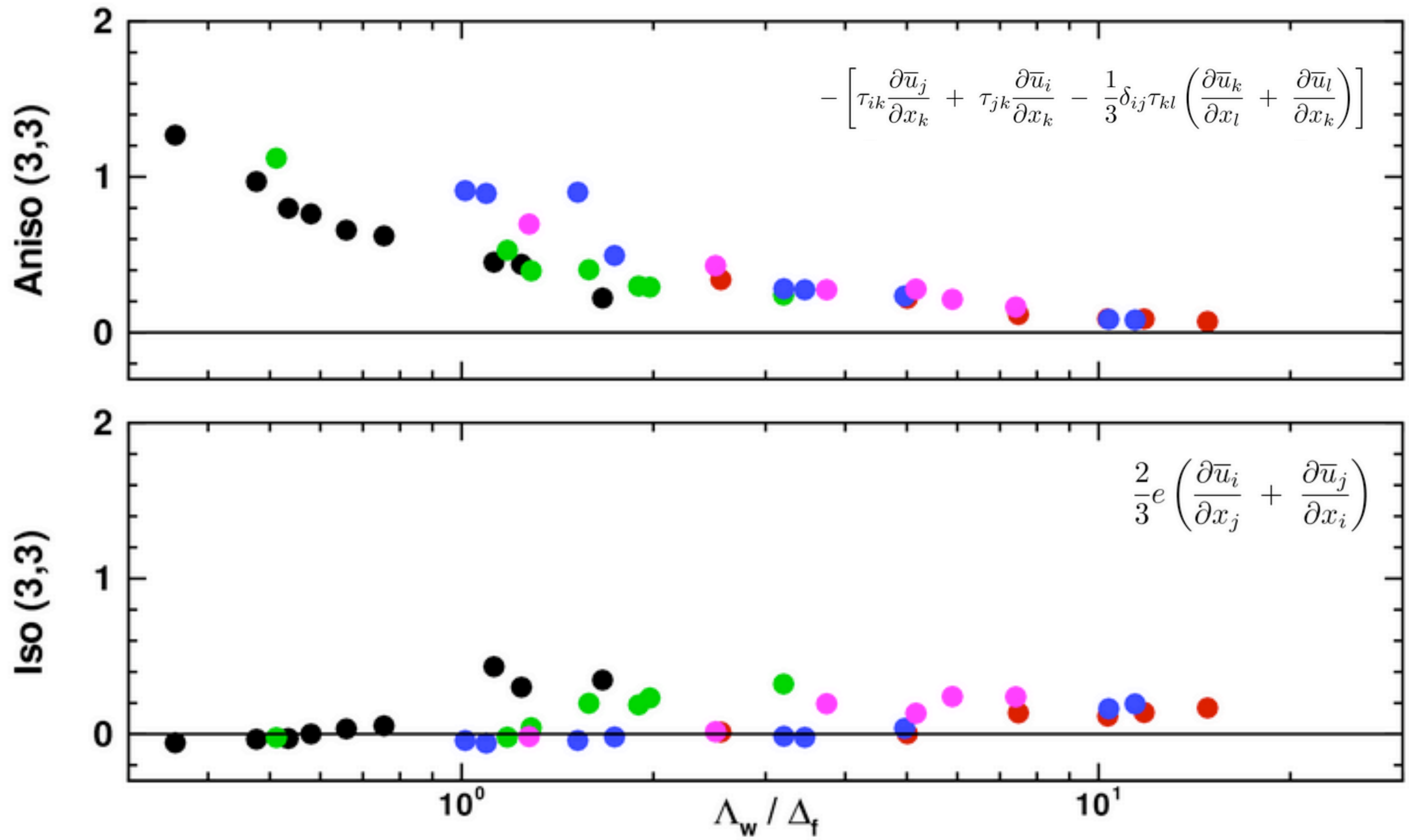
PRODUCTION OF SUBFILTER SCALE FLUX τ_{11}



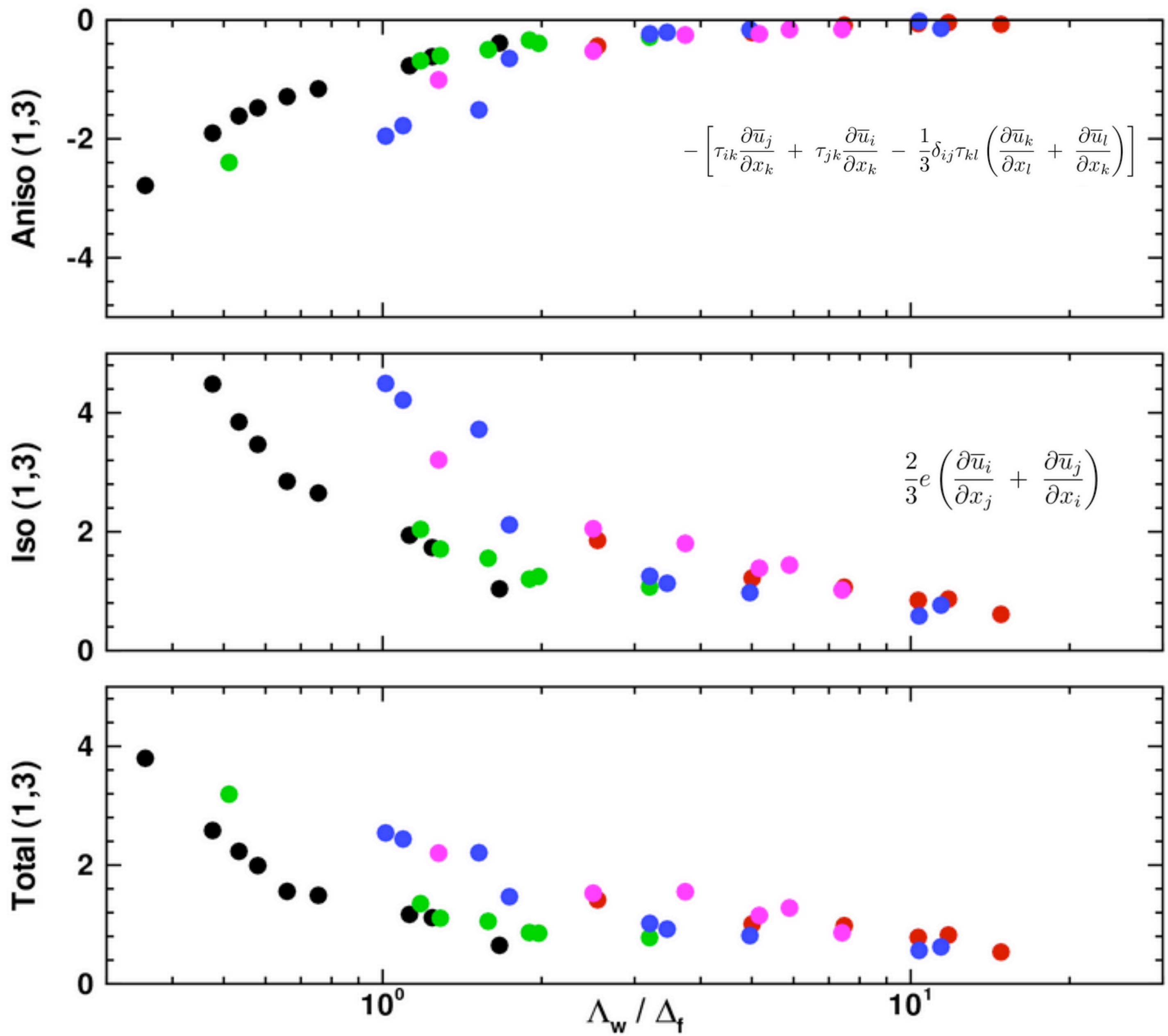


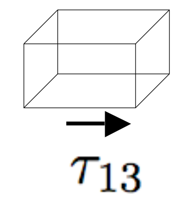
PRODUCTION OF SUBFILTER SCALE FLUX τ_{33}



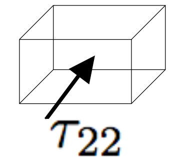


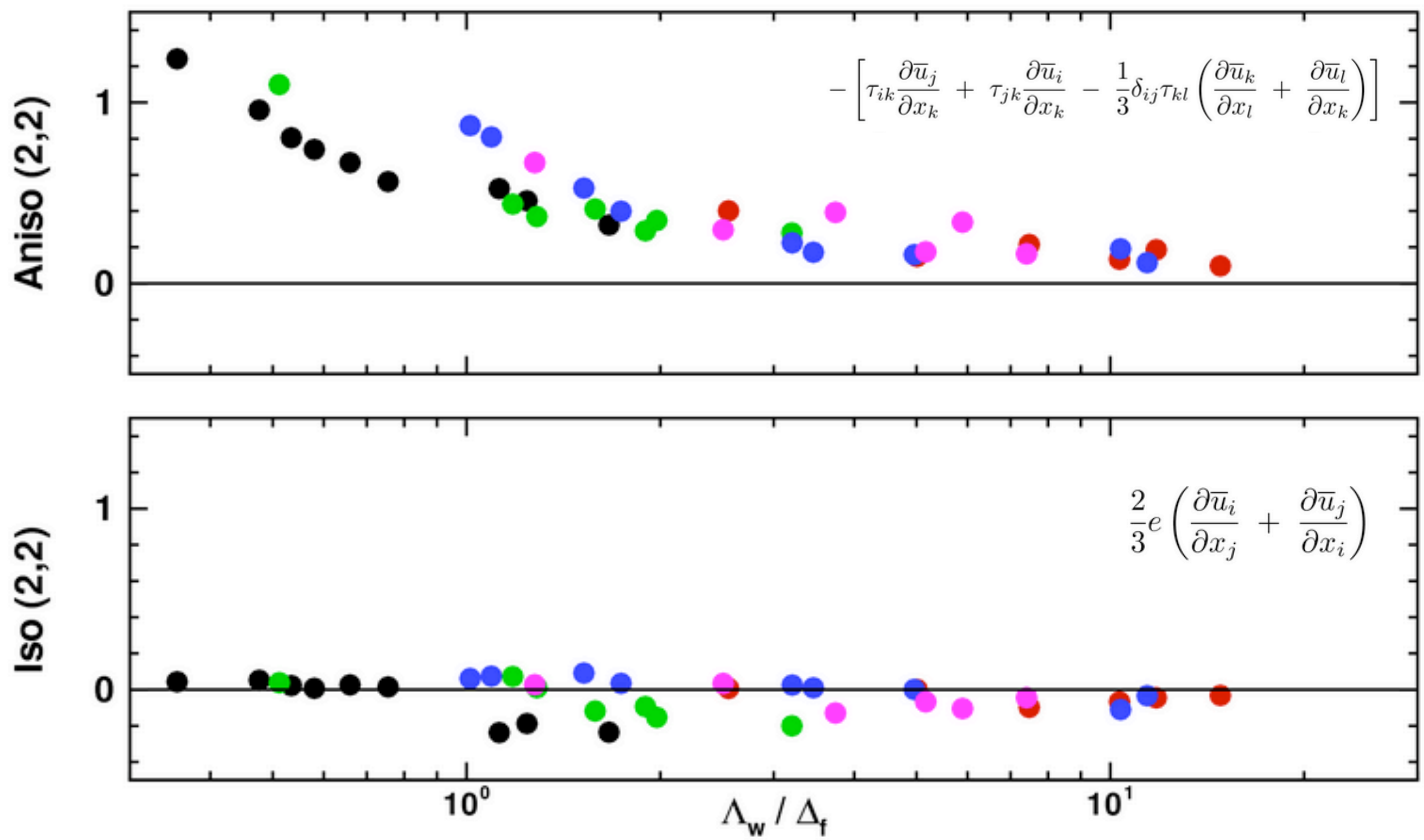
PRODUCTION OF SUBFILTER SCALE FLUX τ_{13}





PRODUCTION OF SUBFILTER SCALE FLUX τ_{22}





VARIATION OF DEVIATORIC STRESS IN LIMIT $\Lambda_w/\triangle_f \to 0$

Steady-state rate equations	Smagorinsky model
$\langle \tau_{11} \rangle = T\left(-2\langle \tau_{13} \rangle \frac{\partial U}{\partial z} + \frac{2}{3}\epsilon\right)$	$\langle \tau_{11} \rangle = 0$
$\langle \tau_{22} \rangle = T\left(\frac{2}{3}\epsilon\right)$	$\langle \tau_{22} \rangle = 0$
$\langle \tau_{33} \rangle = T\left(\frac{2}{3}\epsilon\right)$	$\langle \tau_{33} \rangle = 0$
$\langle \tau_{13} \rangle = T\left(\frac{2}{3}e\frac{\partial U}{\partial z} - \langle \tau_{33} \rangle \frac{\partial U}{\partial z}\right)$	$\langle \tau_{13} \rangle = T\left(\frac{2}{3}e\frac{\partial U}{\partial z}\right)$

Steady-state rate equations

Smagorinsky model

WHAT ABOUT SCALARS?

RATE EQUATIONS FOR SUBGRID SCALAR FLUX

- **What are the parent equations for subgrid-scale scalar flux?**

$$f_i = \overline{u_i c} - \overline{u}_i \overline{c}$$

$$\begin{aligned}\frac{Df_i}{Dt} = \; & -\frac{2}{3} e \frac{\partial \overline{c}}{\partial x_i} \\ & - f_j \frac{\partial \overline{u}_i}{\partial x_j} + \tau_{ij} \frac{\partial \overline{c}}{\partial x_j} \\ & + \frac{1}{\rho}\left(\overline{p \frac{\partial c}{\partial x_i}} - \overline{p} \frac{\partial \overline{c}}{\partial x_i} \right) \\ & + \text{transport} + \text{buoyancy}\end{aligned}$$

Isotropic production

Pressure destruction

Anisotropic production

RATE EQUATIONS FOR SUBGRID SCALAR FLUX

- **What are the parent equations for subgrid-scale scalar flux?**

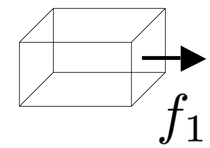
$$f_i = \overline{u_i c} - \overline{u}_i \overline{c}$$

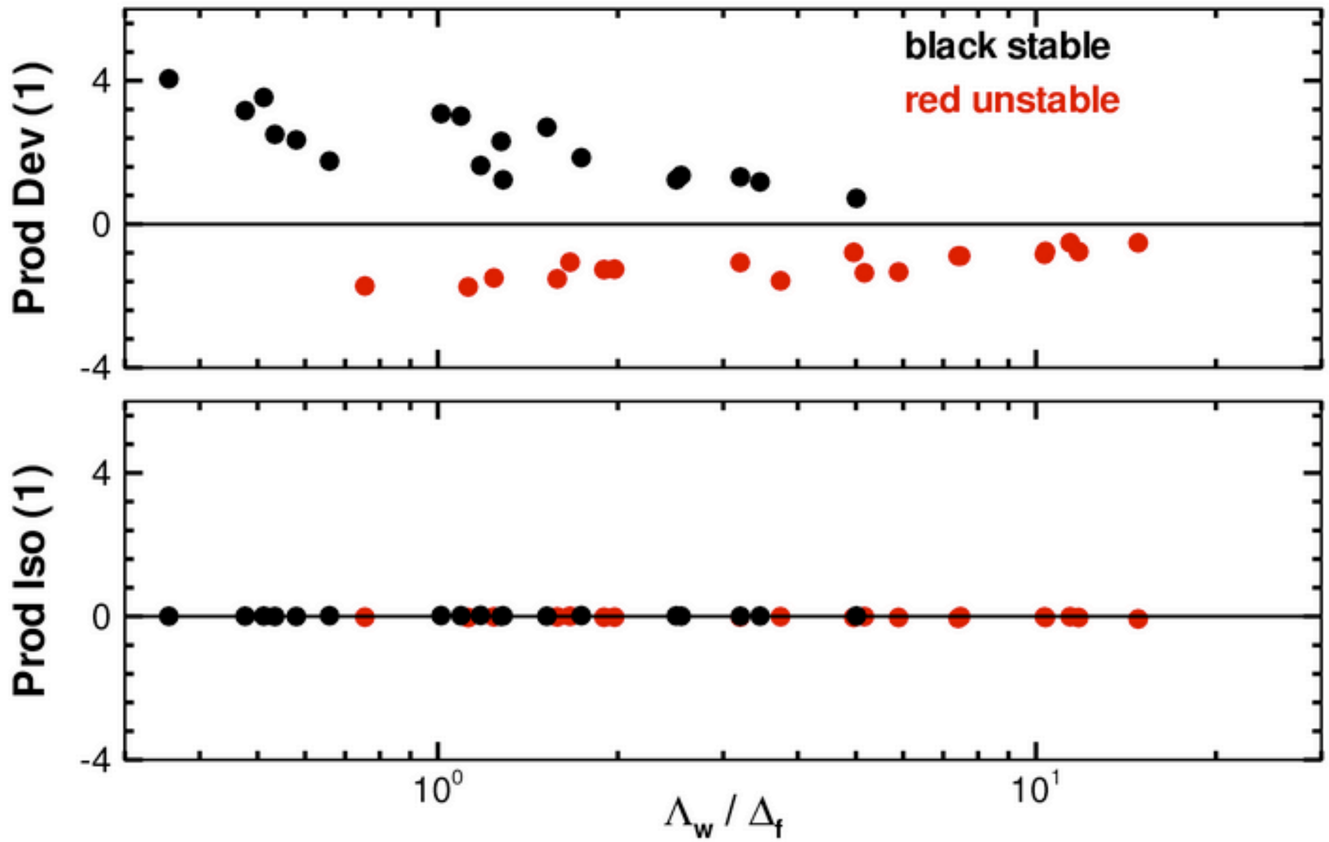
$$\begin{aligned}
\cancelto{0}{\frac{D f_i}{D t}} = & -\frac{2}{3} e \frac{\partial \overline{c}}{\partial x_i} \\
& \cancelto{0}{- f_j \frac{\partial \overline{u}_i}{\partial x_j} + \tau_{ij} \frac{\partial \overline{c}}{\partial x_j}} \\
& + \frac{1}{\rho} \left(\overline{p \frac{\partial c}{\partial x_i}} - \overline{p} \frac{\partial \overline{c}}{\partial x_i} \right) \\
& + \cancelto{0}{\text{transport}} + \cancelto{0}{\text{buoyancy}}
\end{aligned}$$

Eddy viscosity model

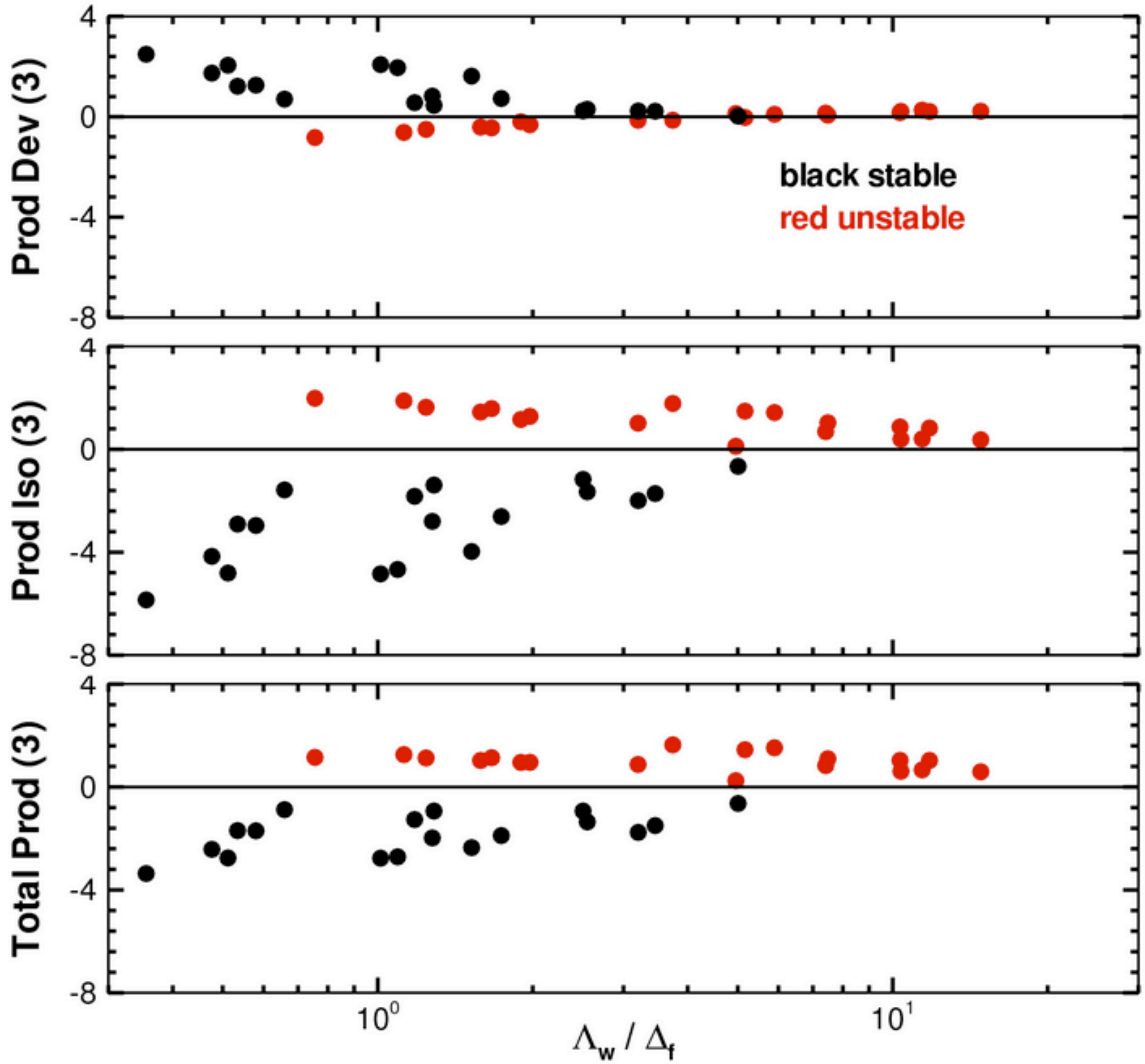
$$\boxed{f_i = -\nu_h \frac{\partial \overline{c}}{\partial x_i} \qquad \nu_h = \frac{2 c_h \Delta_f \sqrt{e}}{3}}$$

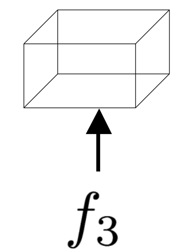
PRODUCTION OF SUBFILTER SCALE SCALAR FLUX f_1





PRODUCTION OF SUBFILTER SCALE SCALAR FLUX f_3



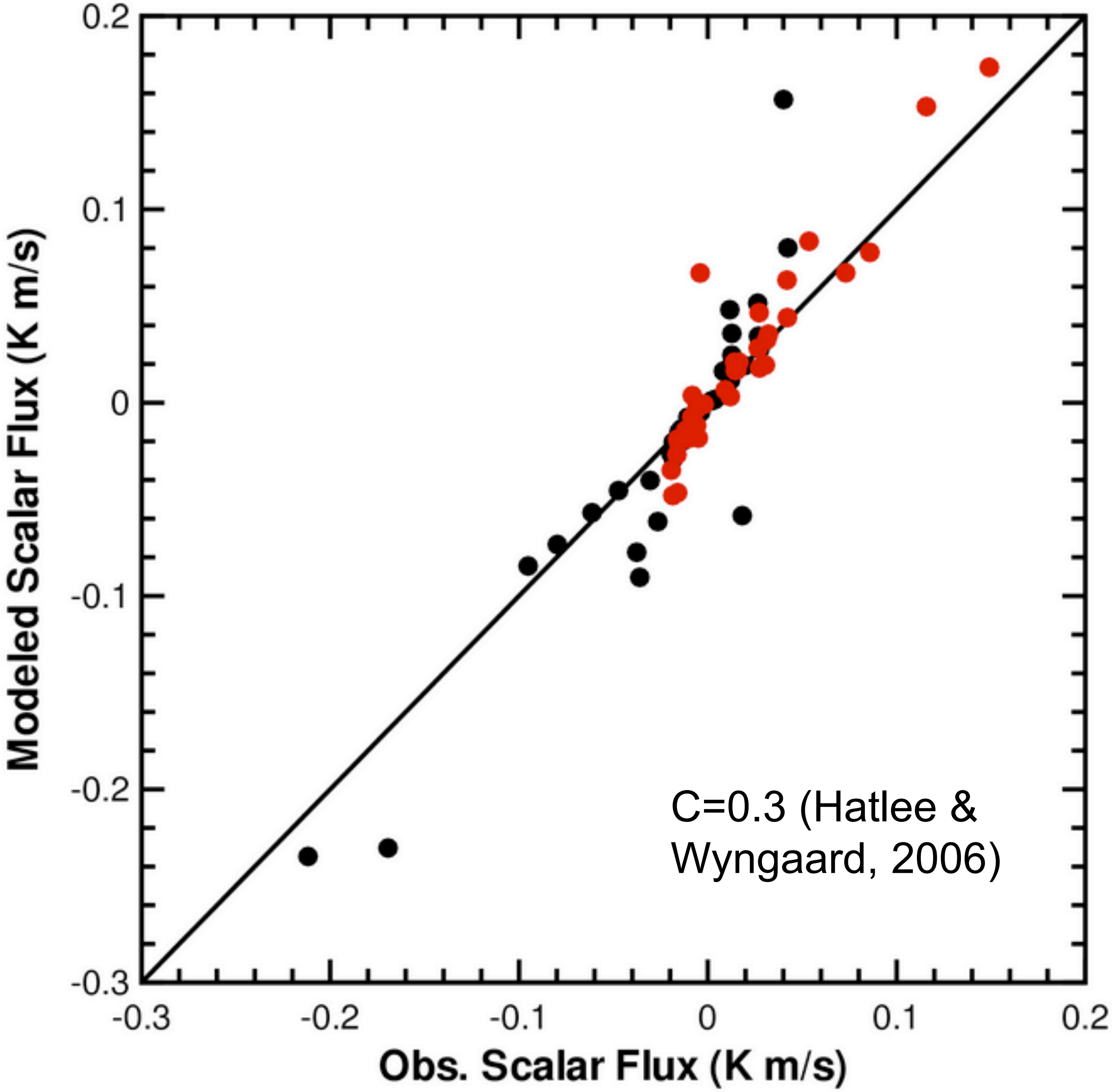


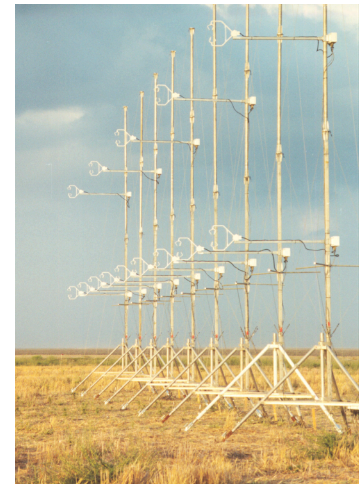
SUBGRID-SCALE SCALAR FLUX

Comments:

- Net horizontal scalar flux $f_1 = \langle \overline{uc} - \overline{u}\,\overline{c} \rangle \neq 0$ even for horizontally homogeneous PBLs, $i.e.,$ $\dfrac{\partial}{\partial x}\langle C \rangle = 0$
- Tilting of vertical flux by vertical shear is important $f_1 \sim -f_3 \dfrac{\partial \overline{u}}{\partial z} T$
- No eddy viscosity model can capture anisotropic production

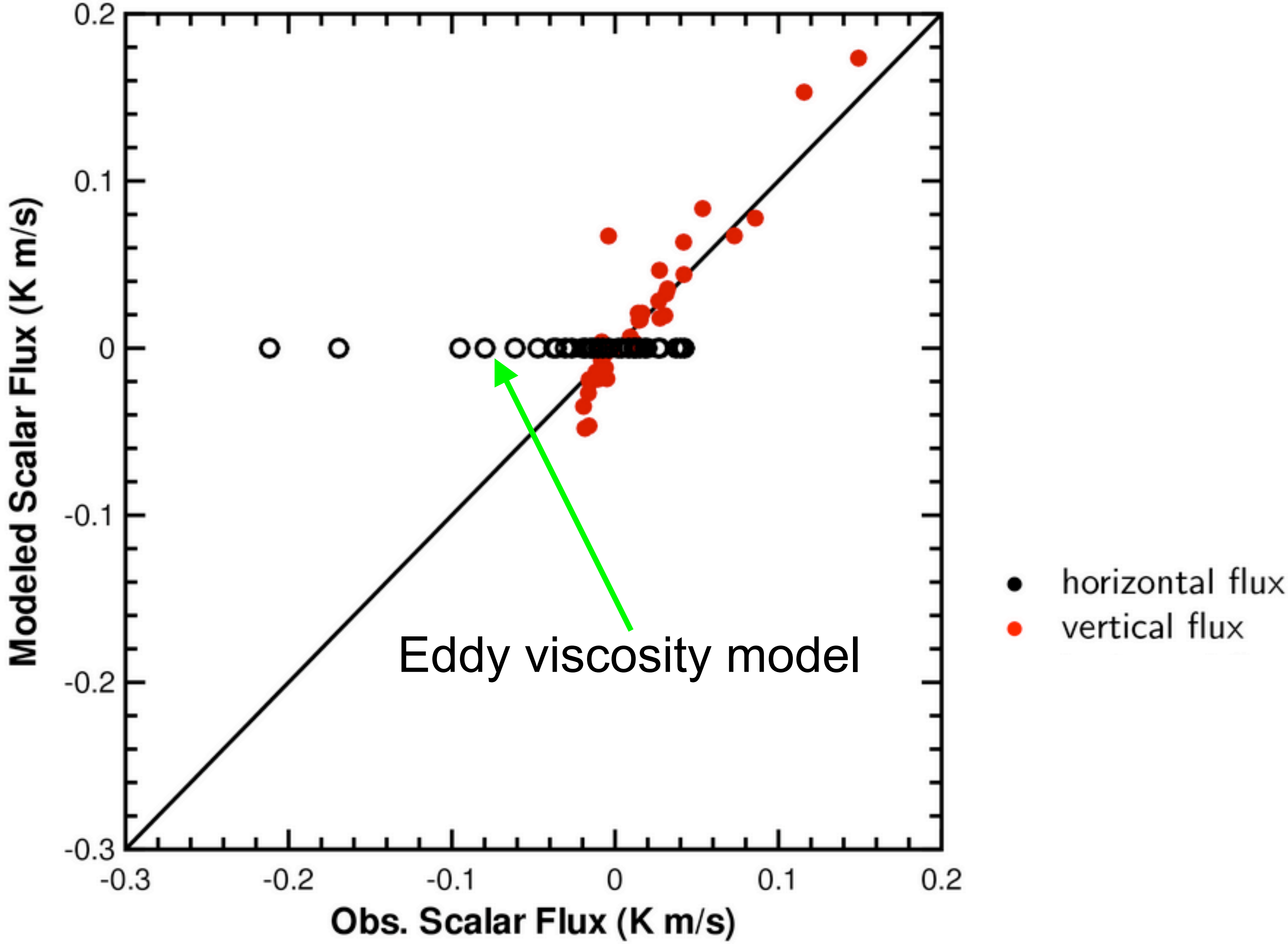
SFS SCALAR FLUXES IN HATS





● horizontal flux
● vertical flux

SFS SCALAR FLUXES IN HATS



TESTING OTHER TERMS ....

SUBFILTER-SCALE PRESSURE DESTRUCTION

Momentum

$$-\frac{1}{\rho}\left[\overline{p\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)}-\overline{p}\left(\frac{\partial \overline{u}_i}{\partial x_j}+\frac{\partial \overline{u}_j}{\partial x_i}\right)\right] = -\frac{\tau_{ij}\sqrt{e}}{C_m\,\triangle_f}$$

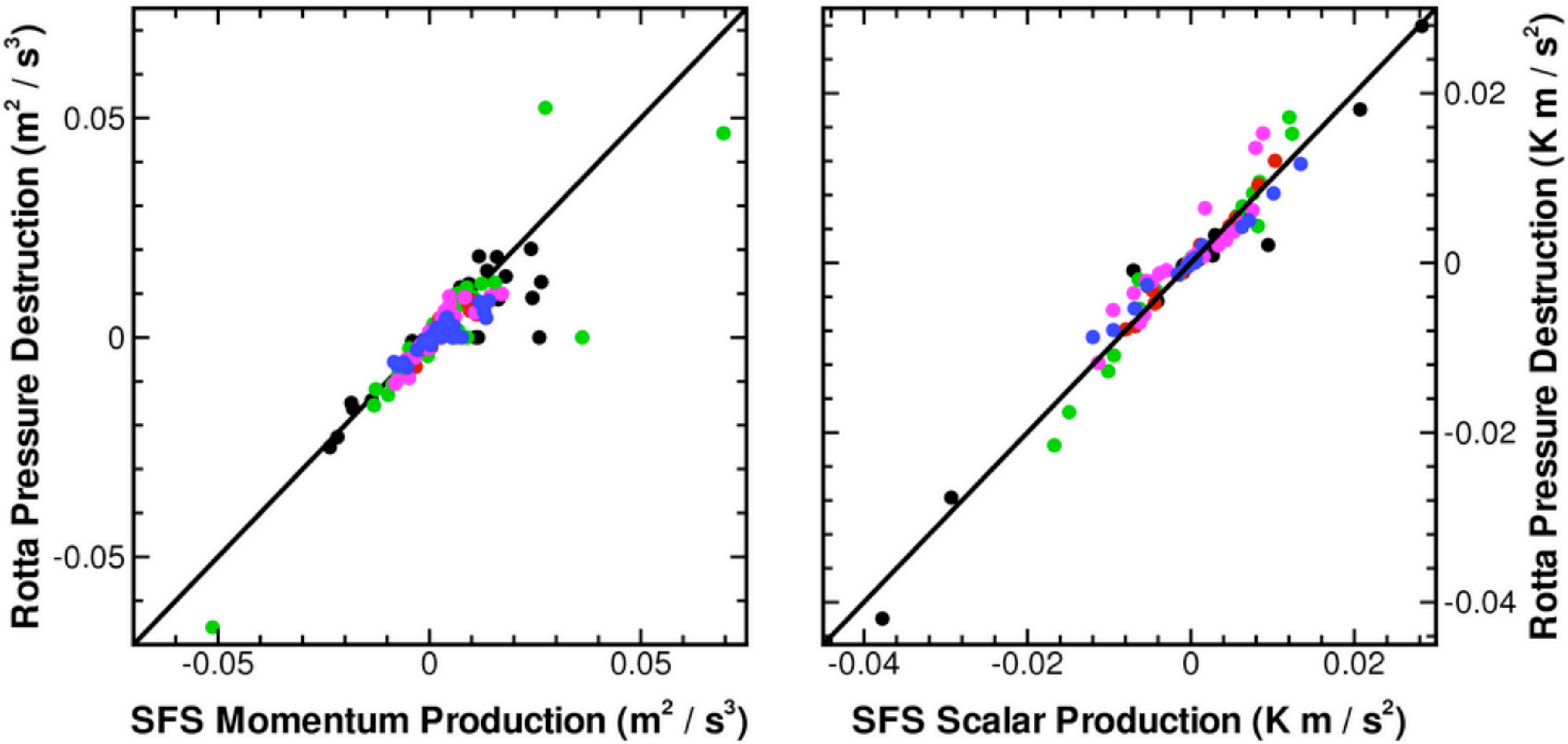
$$+\frac{1}{\rho}\left(\overline{p\frac{\partial c}{\partial x_i}}-\overline{p}\frac{\partial \overline{c}}{\partial x_i}\right) = -\frac{f_i\sqrt{e}}{C_s\,\triangle_f}$$

Scalar

CHATS PRESSURE SENSOR (Steven Oncley)

AHATS (2008) ``HORIZONTAL ARRAY” OF PRESSURE SENSORS

VALIDATION OF ROTTA MODEL FOR MOMENTUM AND SCALARS



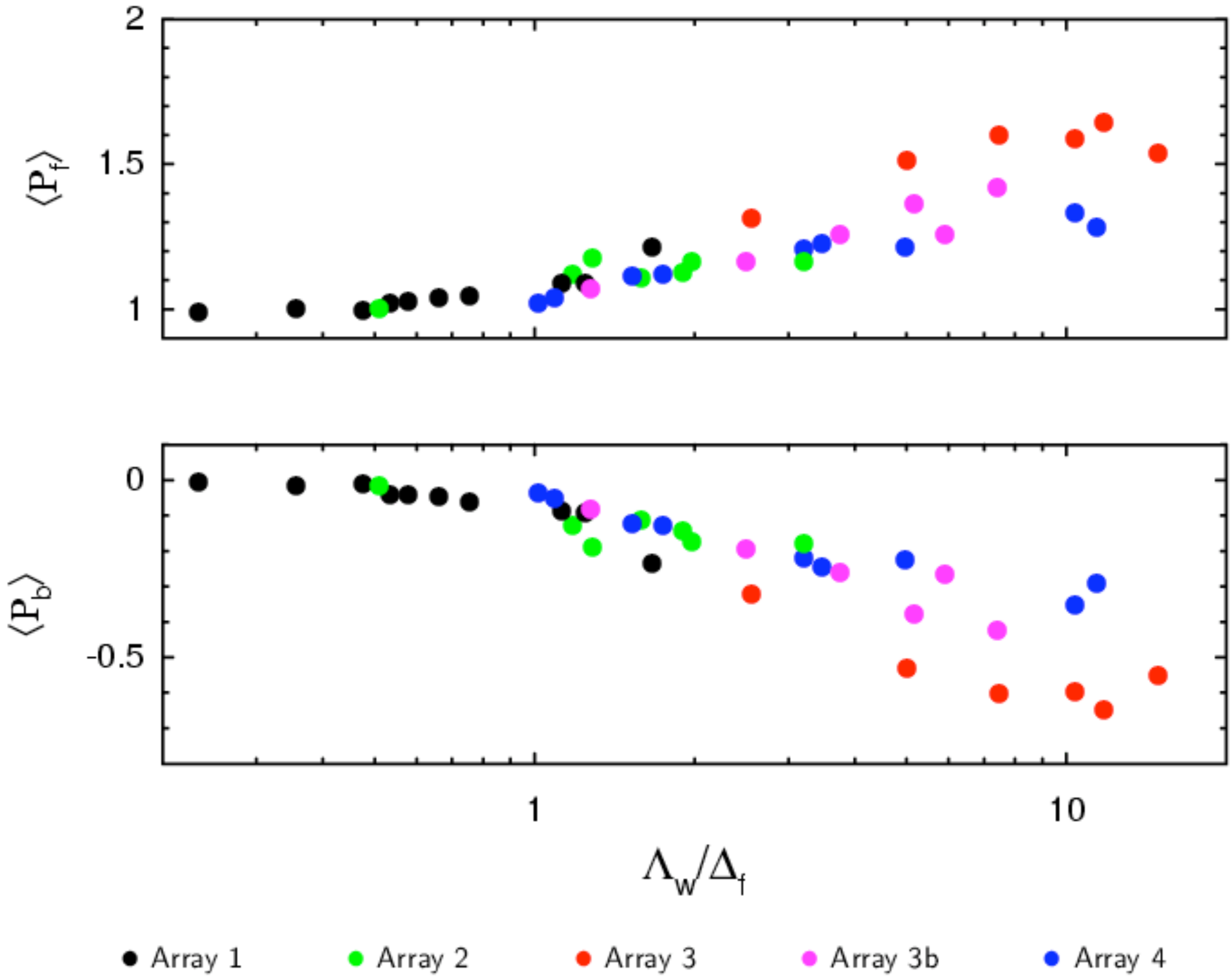
$$Production \approx Destruction$$

Decomposition of SFS Production into Forwardscatter and Backscatter

$$P = -\mathcal{T}_{ij} S_{ij} \quad P_f = (P + |P|)/2 \quad P_b = (P - |P|)/2$$

Decomposition of SFS Production into Forwardscatter and Backscatter

$$P = -\mathcal{T}_{ij} S_{ij} \qquad P_f = (P + |P|)/2 \qquad P_b = (P - |P|)/2$$



SUMMARY

- LES is being applied to a richer set of boundary layer flows because of advances in parallel computing
- Subgrid-scale parameterizations in LES need to be validated/improved for geophysical applications
- Multi-point measurements from the HATS field campaigns compliment our ability to compute
  - Evaluation of subgrid scale models with high Re data
  - Rate equations provide insight into SGS dynamics
  - Importance of anisotropic production for stress and scalar especially for $\Lambda_w/\Delta_f \sim \mathcal{O}(1)$ or less
  - Data highlights the shortcomings of an eddy viscosity approach

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