Effects of Local Conditions on Smagorinsky and Dynamic Coefficients for LES of Atmospheric Turbulence

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SGS models in the atmospheric boundary layer

- Simplest approach: Smagorinsky eddy viscosity model (MWR – 1963)

$$\tau_{ij}^{smag} = -2\nu_T \widetilde{S}_{ij} \qquad \nu_T = \ell^2 |\widetilde{\mathbf{S}}| = (c_s \Delta)^2 |\widetilde{\mathbf{S}}|$$

- Three main (and possibly related) problems:

1) Cannot afford to resolve viscous layer

- First vertical grid points: $\Delta \sim L$ (integral scale)

Mason (QJRMS – 1994), Meneveau and Katz (ARFM – 2000)

2) Effect of mean shear:

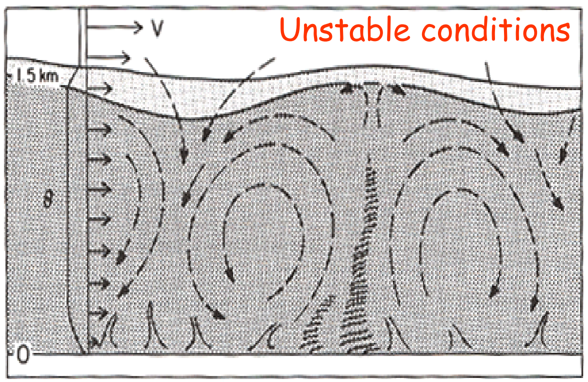
- ν_T proportional to resolved **turbulent** velocity gradients
- In regions of strong mean shear, ν_T is overestimated

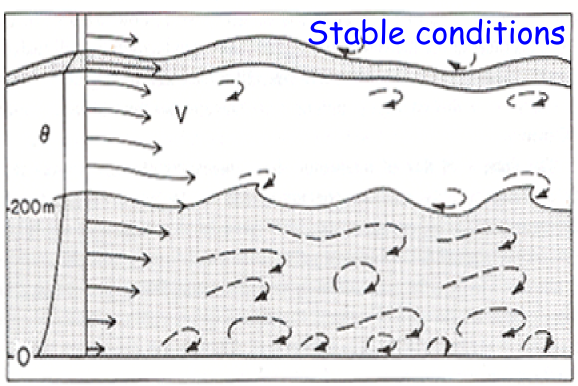
Schumann (JCP - 1975), Mason (QJRMS – 1994)

3) Buoyancy:

- Affects both the integral scale and the energy balance
- Also affects the structure of the turbulence

Mason (QJRMS, 1994), Canuto and Cheng (PoF – 1997)





Figures from Wyngaard (BLM-1990)

Motivation and objectives

- **Motivation:** improve dynamic SGS models (Germano et al., PoF - 1991) in atmospheric boundary layer simulations by introducing dependence on local flow conditions

- **Final goal**: reformulate the dynamic Smagorinsky SGS model based on averages conditioned on the local structure of turbulence (instead of volume or time averages)

$$\left(c_s^2\right)^{dyn} = \frac{\langle L_{ij}M_{ij} | \Pi_1, \Pi_2, \ldots\rangle}{\langle M_{mn}M_{mn} | \Pi_1, \Pi_2, \ldots\rangle}$$

- **First step:** use a priori analysis of experimental data obtained in the atmospheric surface layer to define (identify) a set of physically relevant dimensionless parameters

$$c_s^2 = f(\Pi_1, \Pi_2, \ldots)$$

Characterization of the local structure of turbulence

- Use 6 dimensionless parameters locally defined:

1. Atmospheric stability

Majda and Shefter (JFM - 1998)

$$Ri = \frac{-\mathbf{g}\cdot\nabla\widetilde{T}}{\widetilde{T}(|\widetilde{\mathbf{S}}|^2 + |\widetilde{\omega}|^2)}$$

Temperature gradient

$$Ri^* = \mathrm{erf}(Ri)$$

2. Distance from the surface

Kleissl et al. (JAS - 2003)

$$\Delta/z$$

Distance from the surface

Filter width

3. Strain state (type of deformation)

Lund and Rogers (PoF - 1994)

$$S^* = \frac{-12\sqrt{3}\mathrm{Det}(\widetilde{\mathbf{S}})}{|\widetilde{\mathbf{S}}|^3}$$

4. Balance between vorticity and strain

Hunt et al. (1998)

$$Q^* = \frac{|\widetilde{\omega}|^2 - |\widetilde{\mathbf{S}}|^2}{|\widetilde{\omega}|^2 + |\widetilde{\mathbf{S}}|^2}$$

Strain rate magnitude

Vorticity magnitude

5. Vortex stretching magnitude

$$V^* = \frac{3|\widetilde{\mathbf{S}}\cdot\widetilde{\omega}|^2}{|\widetilde{\omega}|^2|\widetilde{\mathbf{S}}|^2}$$

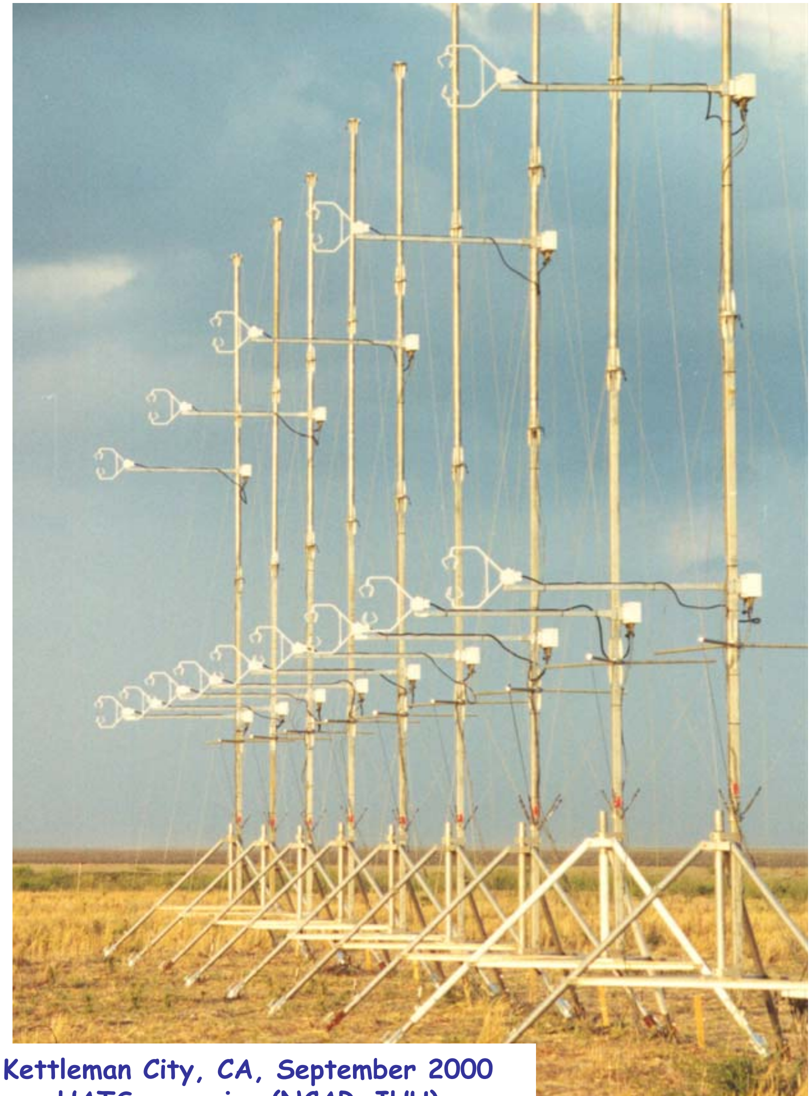
Magnitude of vortex stretching vector

6. Effectiveness of vortex stretching

$$W^* = \frac{\widetilde{\omega}\cdot(\widetilde{\mathbf{S}}\cdot\widetilde{\omega})}{|\widetilde{\omega}||\widetilde{\mathbf{S}}\cdot\widetilde{\omega}|}$$

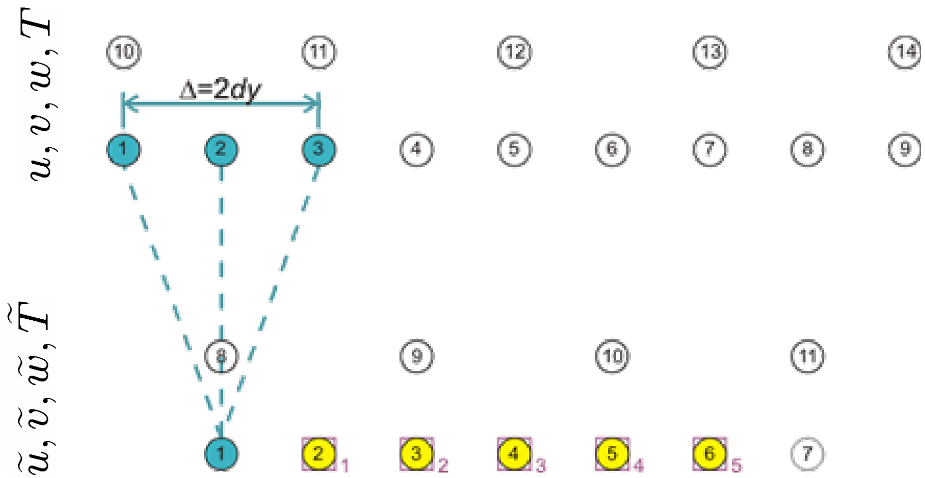
Working hypothesis $c_s^2 = f(Ri^*, \Delta/z, S^*, Q^*, V^*, W^*)$

The HATS data set



Kettleman City, CA, September 2000
HATS campaign (NCAR-JHU)
(see Horst *et al.*, JAS - 2004)

- Apply 2D filter (Gaussian + Box):



- Determine c_s^2 by requiring the model to predict the correct dissipation:

Measured SGS dissipation

$$c_s^2(\Pi_1, \Pi_2, \ldots) = \frac{\langle -\tau_{ij}\tilde{S}_{ij} | \Pi_1, \Pi_2, \ldots\rangle}{\langle 2\Delta^2 |\tilde{S}|\tilde{S}_{ij}\tilde{S}_{ij} | \Pi_1, \Pi_2, \ldots\rangle}$$

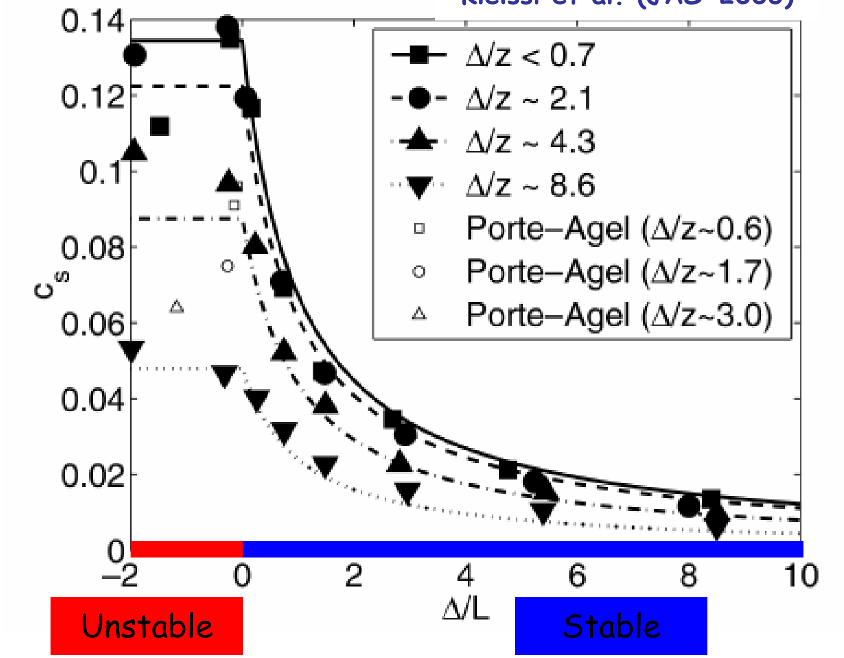
Smagorinsky dissipation

Effects of atmospheric stability

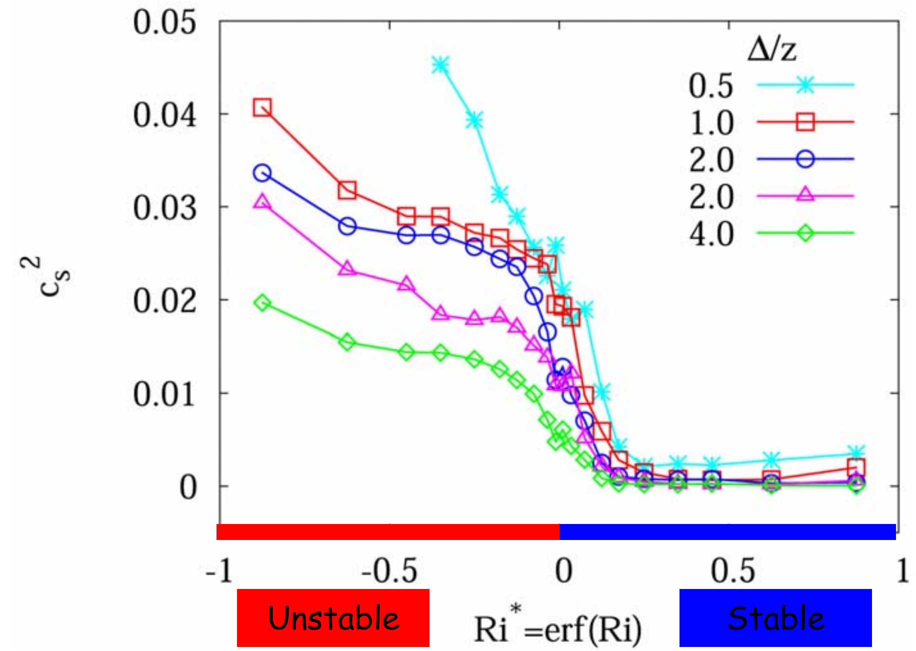
Characterized by Obukhov length (fluxes averaged over 6.8 minute periods)

Characterized by local Richardson number (locally defined at every point)

Kleissl et al. (JAS-2003)



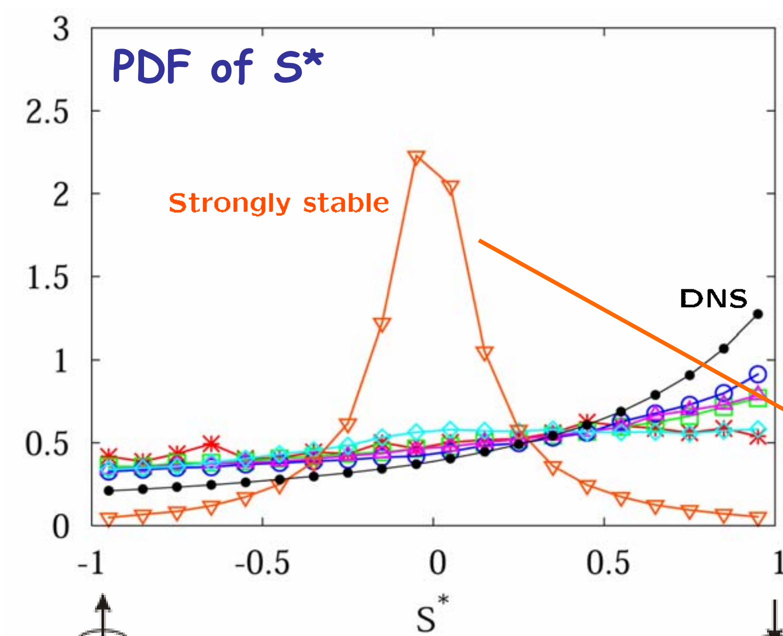
$c_s^2(Ri^*, \Delta/z)$



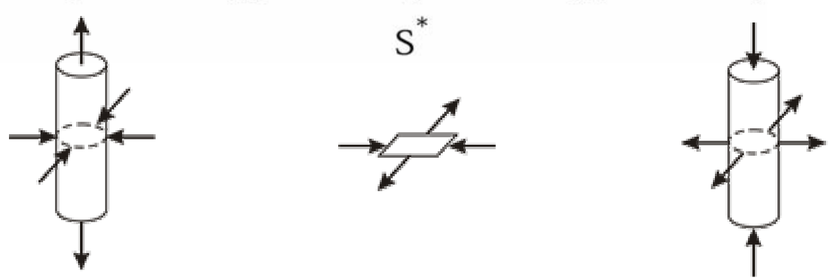
Local Richardson number captures the expected effects of stability

Atmospheric stability and strain state

$$S^* = \frac{-12\sqrt{3}\mathrm{Det}(\tilde{\mathrm{S}})}{|\tilde{\mathrm{S}}|^3}$$



$-1.00 \leq Ri^* < -0.30$	Strongly unstable	
$-0.30 \leq Ri^* < -0.02$	Unstable	
$-0.02 \leq Ri^* < 0.00$	Weakly unstable	
$0.00 \leq Ri^* < +0.03$	Weakly stable	
$+0.03 \leq Ri^* < +0.15$	Stable	
$+0.15 \leq Ri^* < +1.00$	Strongly stable	
—	Neutral DNS	



$S^* = -1$ Axisymmetric Contraction

$S^* = 0$ Plane Shear

$S^* = 1$ Axisymmetric Extension

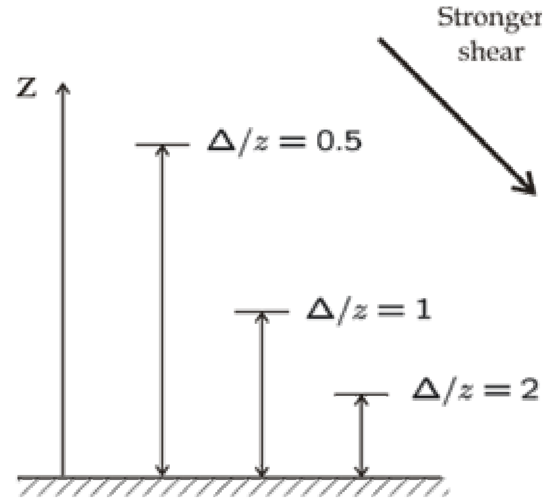
Important conclusion:

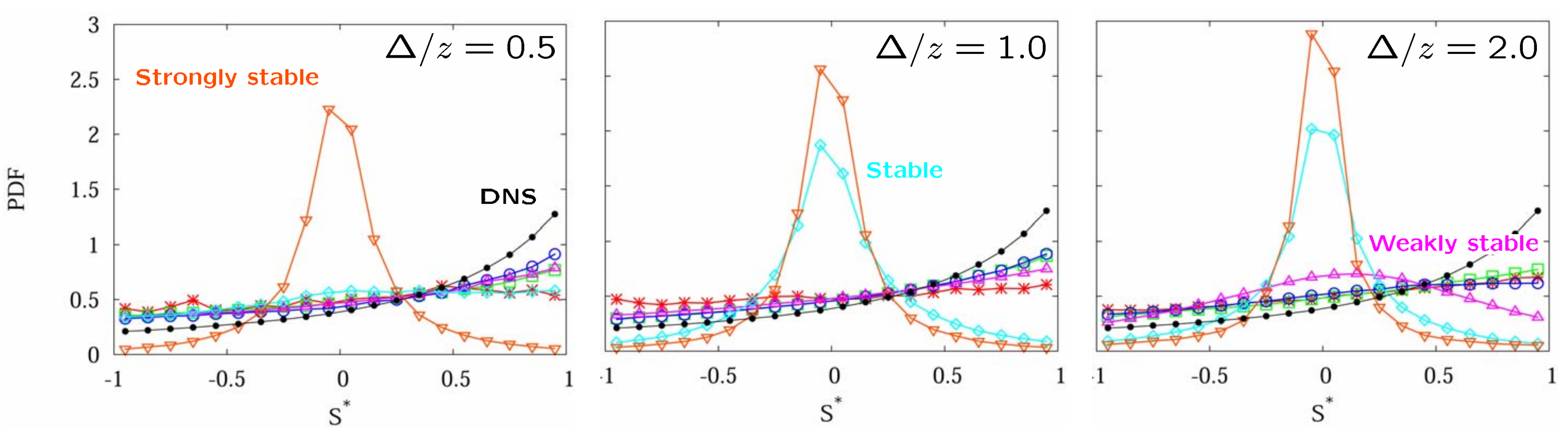
Under strongly stable conditions buoyancy suppress turbulent fluctuations and the mean shear dominates the distribution of local structure of the velocity gradient tensor.

Atmospheric stability and distance from the surface

Effect of relative importance between mean and turbulent velocity gradients on the local structure of the turbulence

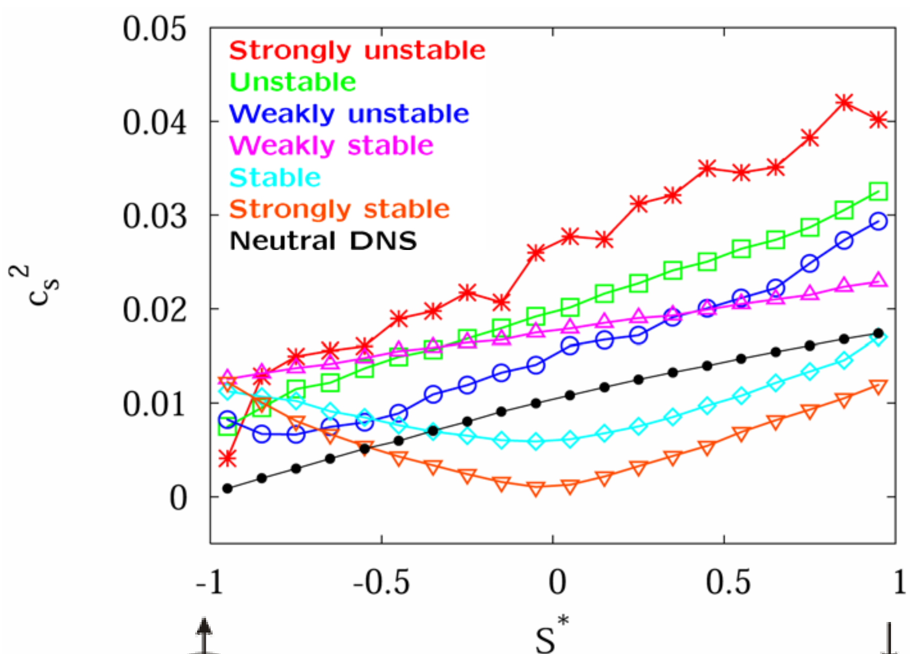
$$S^* = \frac{-12\sqrt{3}\mathrm{Det}(\tilde{\mathrm{S}})}{|\tilde{\mathrm{S}}|^3}$$

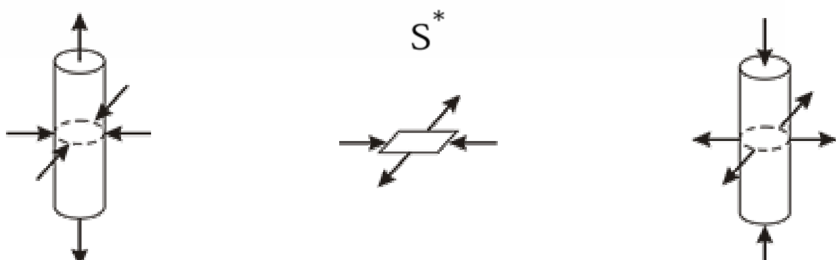




Effects of local strain state

$$c_s^2(S^*, Ri^*, \Delta/z = 1)$$

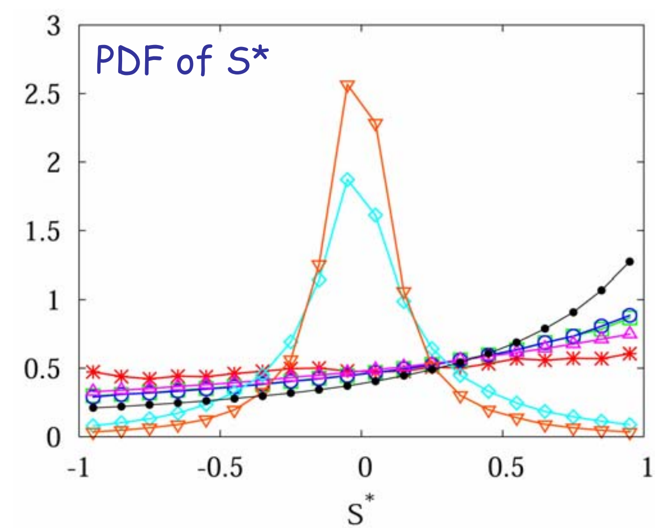




$S^* = -1$	$S^* = 0$	$S^* = 1$
Axisymmetric Contraction	Plane Shear	Axisymmetric Extension

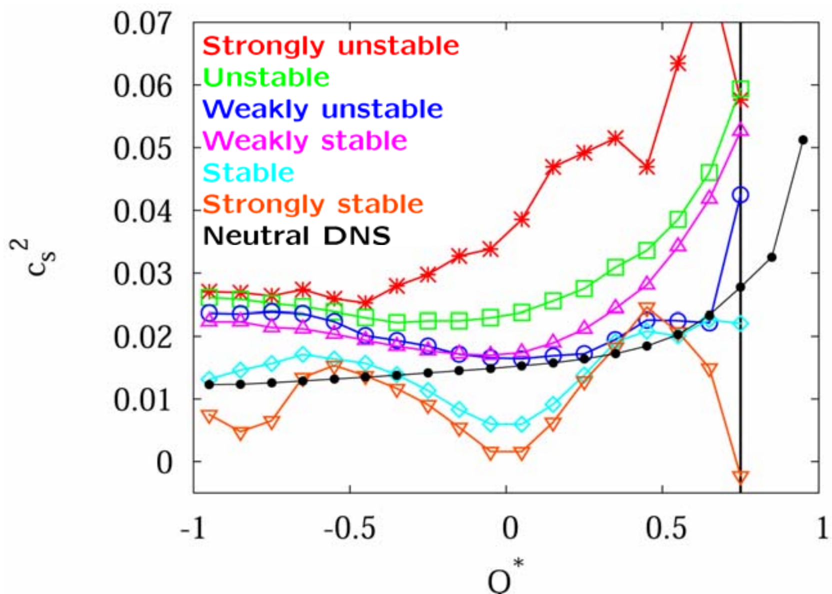
$$S^* = \frac{-12\sqrt{3}\mathrm{Det}(\widetilde{\mathbf{S}})}{|\widetilde{\mathbf{S}}|^3}$$

$$c_s^2(S^*, Ri^*) = \frac{\langle -\tau_{ij}\widetilde{S}_{ij} |\ S^*, Ri^*\rangle}{\langle 2\Delta^2 |\widetilde{S}|\widetilde{S}_{ij}\widetilde{S}_{ij} |\ S^*, Ri^*\rangle}$$

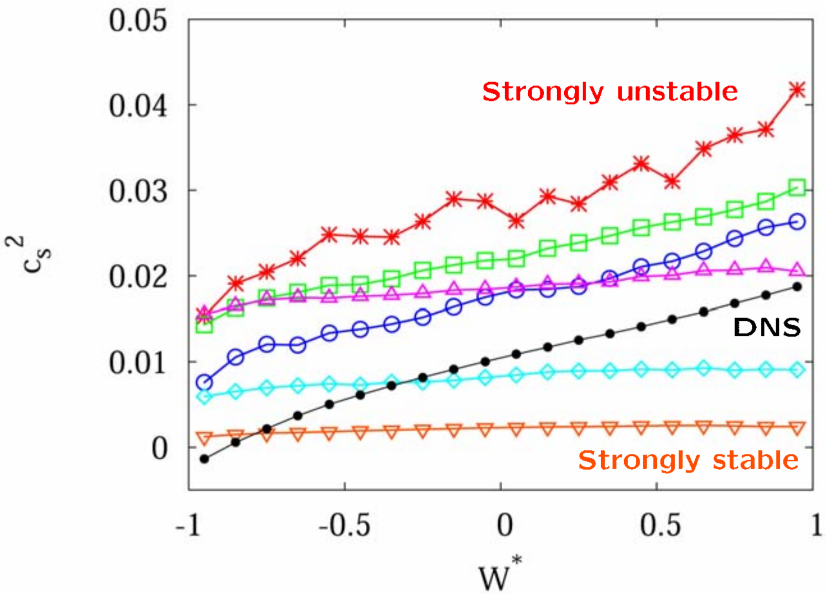


Effects of vorticity and vortex stretching

$$c_s^2(Q^*, Ri^*, \Delta/z = 1)$$



$$c_s^2(W^*, Ri^*, \Delta/z = 1)$$



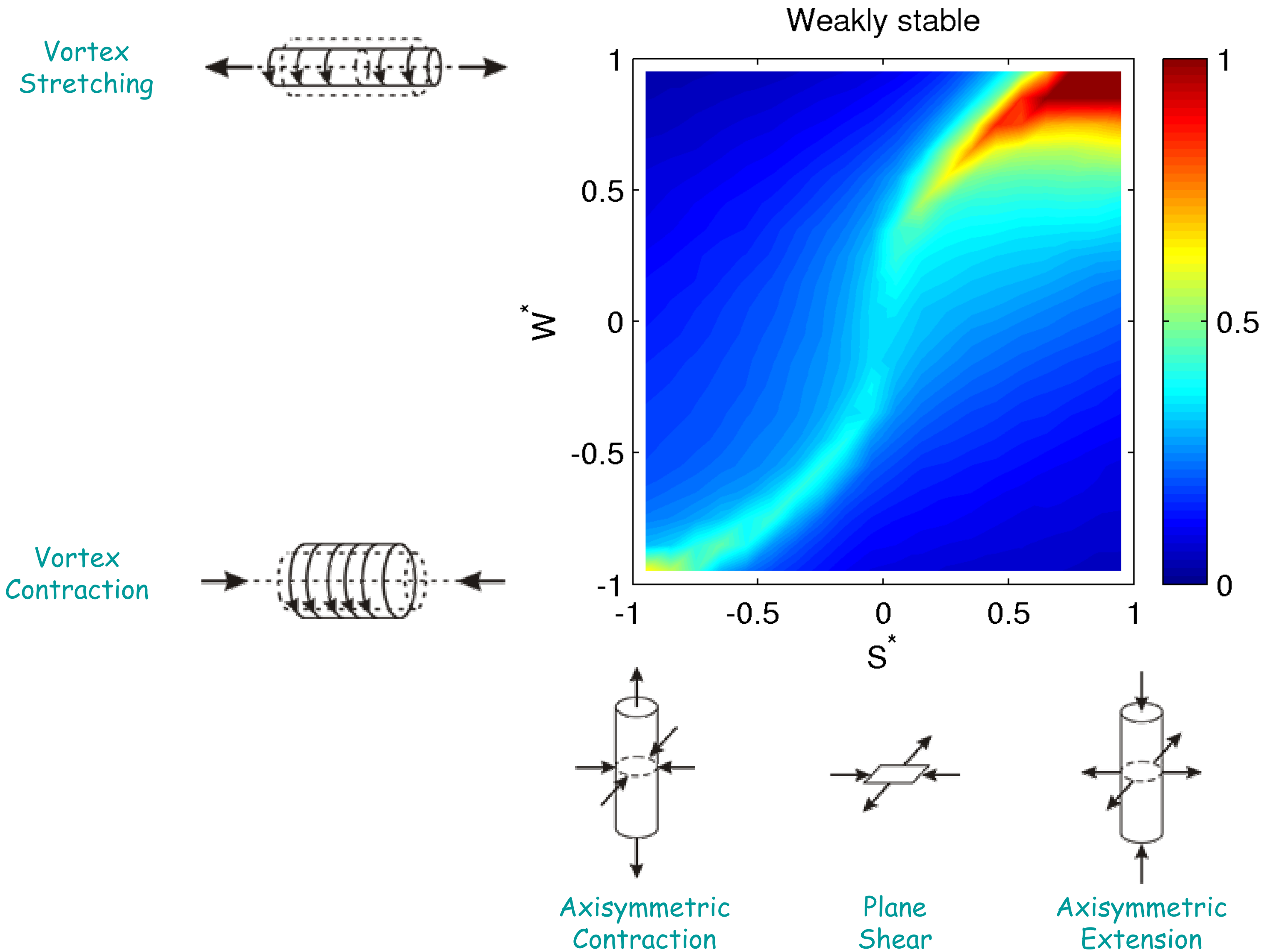
Strain dominated | Vorticity dominated

$$Q^* = \frac{|\widetilde{\omega}|^2 - |\widetilde{\mathrm{S}}|^2}{|\widetilde{\omega}|^2 + |\widetilde{\mathrm{S}}|^2}$$

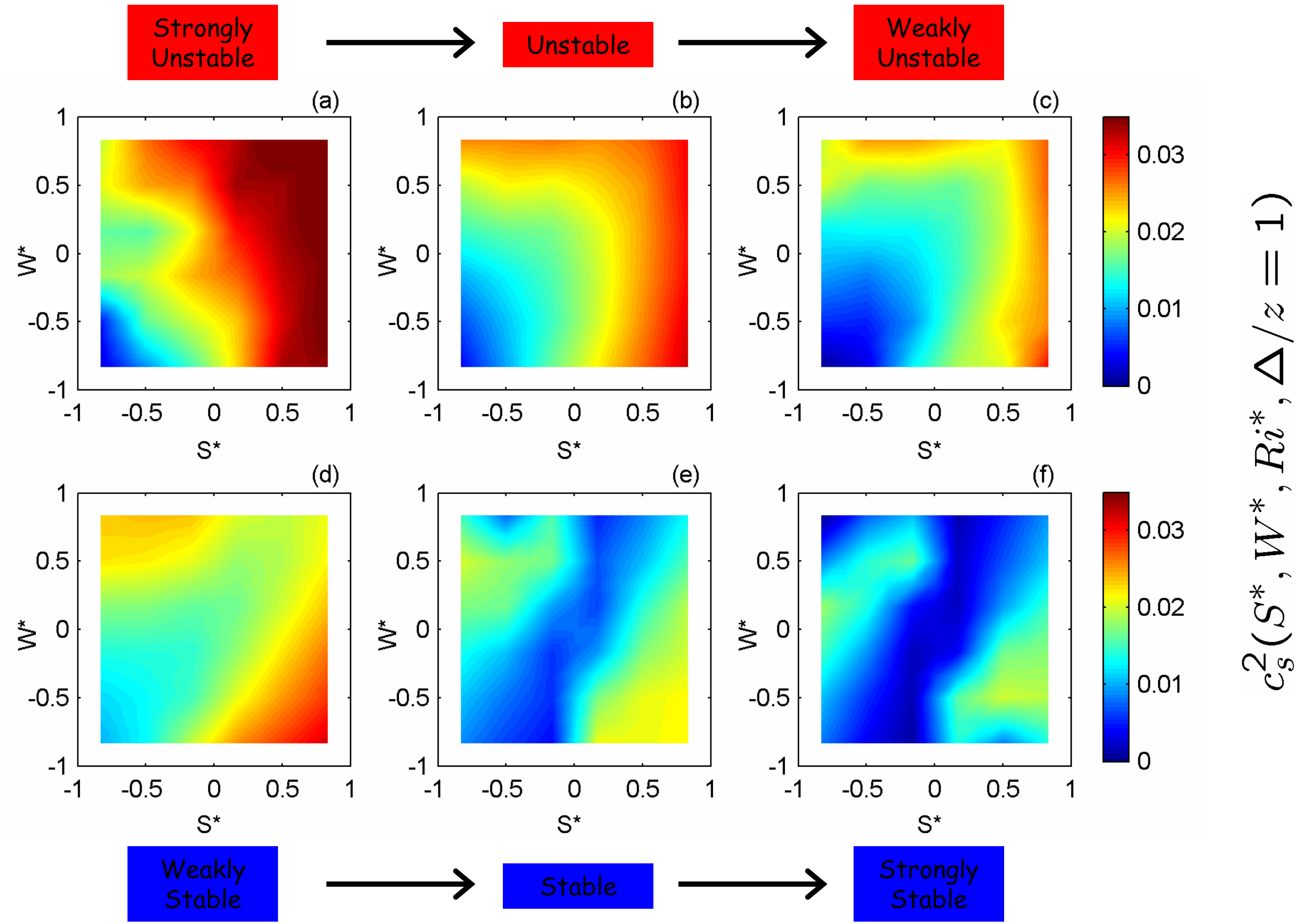
Vortex compressing | Vortex stretching

$$W^* = \frac{\widetilde{\omega} \cdot (\widetilde{\mathrm{S}} \cdot \widetilde{\omega})}{|\widetilde{\omega}||\widetilde{\mathrm{S}} \cdot \widetilde{\omega}|}$$

Joint PDFs of S* and W*



Results from HATS: c_s dependence on S* and W*



Summary of *a priori* results

- Parameters proposed have important effect on the optimal value of the Smagorinsky coefficient
- Functional dependences not amenable to factorization

  i.e. $c_s^2 = f(\Pi_1, \Pi_2)$ $\quad$ $c_s^2 \stackrel{?}{=} f_1(\Pi_1) f_2(\Pi_2)$
- For more details: Chamecki et al. (JAS – 2007)

- Proposed approach:

  - Assume $c_s^2 = f(\mathcal{S})$ $\quad$ $\mathcal{S}$ is a set of parameters describing the local structure of the turbulence

  - Dynamically determine the functional dependence using the Germano identity (Germano et al., PoF - 1991)

Germano identity and dynamic model

- SGS at grid-filter scale (Δ): $\tau_{ij} = \widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j$
- SGS at test-filter scale ($\gamma\Delta$): $T_{ij} = \overline{\widetilde{u_i u_j}} - \bar{\tilde{u}}_i \bar{\tilde{u}}_j$
- Germano et al (PoF - 1991): $L_{ij} \equiv \overline{\tilde{u}_i \tilde{u}_j} - \bar{\tilde{u}}_i \bar{\tilde{u}}_j = T_{ij} - \bar{\tau}_{ij}$
- Smagorinsky model at both scales:

$$\tau_{ij} = -2(c_s^{\Delta}\Delta)^2 |\tilde{\mathrm{S}}| \tilde{S}_{ij} \qquad\qquad T_{ij} = -2(c_s^{\gamma\Delta}\gamma\Delta)^2 |\bar{\tilde{\mathrm{S}}}| \bar{\tilde{S}}_{ij}$$

- Define error: $\epsilon_{ij} \equiv L_{ij} - (T_{ij} - \bar{\tau}_{ij})$
- Assuming $c_s^{\gamma\Delta} = c_s^{\Delta}$ and minimizing least square error yields:

$$(c_s^{\Delta})^2 = \frac{\langle L_{ij} M_{ij} \rangle}{\langle M_{mn} M_{mn} \rangle}$$

Averages over directions of statistical homogeneity

Proposed use of Germano identity

- Error expression from Germano identity:

$$\epsilon_{ij} \equiv L_{ij} - \left(T_{ij} - \overline{\tau}_{ij}\right) = L_{ij} - 2\Delta^2 \left[(c_s^{\Delta})^2 \overline{|\widetilde{\mathbf{S}}|\widetilde{S}_{ij}} - \gamma^2 (c_s^{\gamma\Delta})^2 |\overline{\widetilde{\mathbf{S}}}|\overline{\widetilde{S}}_{ij} \right]$$

$$(c_s^{\Delta})^2 = [c_s(\widetilde{\mathcal{S}})]^2$$

$$(c_s^{\gamma\Delta})^2 = [c_s(\overline{\widetilde{\mathcal{S}}})]^2$$

NOTE: The local structure at a given point can be different at different filter scales!

$$\widetilde{\mathcal{S}} \neq \overline{\widetilde{\mathcal{S}}}$$

- Iterative procedure:

$$\epsilon = L_{ij} - 2\Delta^2 \left[[c_s^n(\widetilde{\mathcal{S}})]^2 \overline{|\widetilde{\mathbf{S}}|\widetilde{S}_{ij}} - \gamma^2 [c_s^{n+1}(\overline{\widetilde{\mathcal{S}}})]^2 |\overline{\widetilde{\mathbf{S}}}|\overline{\widetilde{S}}_{ij} \right]$$

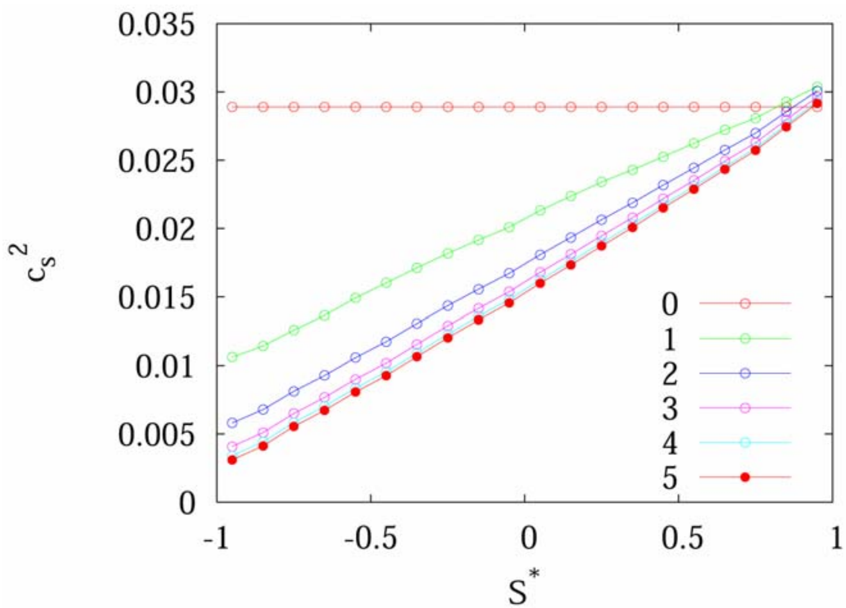
$$[c_s^{n+1}(\overline{\widetilde{\mathcal{S}}})]^2 = \frac{-\left\langle |\overline{\widetilde{\mathbf{S}}}|\overline{\widetilde{S}}_{ij} L_{ij} \mid \overline{\widetilde{\mathcal{S}}} \right\rangle + 2\Delta^2 \left\langle [c_s^n(\widetilde{\mathcal{S}})]^2 \overline{|\widetilde{\mathbf{S}}|\widetilde{S}_{ij}} |\overline{\widetilde{\mathbf{S}}}|\overline{\widetilde{S}}_{ij} \mid \overline{\widetilde{\mathcal{S}}} \right\rangle}{(\gamma\Delta)^2 \left\langle |\overline{\widetilde{\mathbf{S}}}|^4 \mid \overline{\widetilde{\mathcal{S}}} \right\rangle}$$

Averages conditioned on the local structure of the turbulence

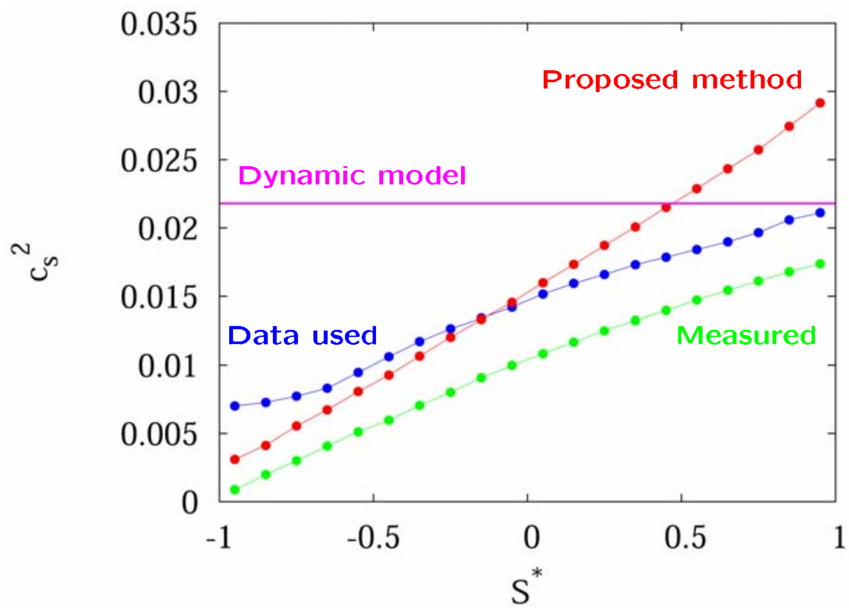
Initial results for DNS of isotropic turbulence

- Simple case: DNS of neutral isotropic turbulence
- Consider only: $c_S^2(\mathcal{S}) = f(S^*)$
- Two main questions to be addressed:

Does it converge?



What does it converge to?



Conclusions and future work

- Identified 6 independent physical dimensionless groups to characterize the local structure of turbulence:
  - 4 to characterize the velocity gradient tensor
  - 1 to characterize buoyancy/atmospheric stratification
  - 1 to characterize distance from a solid boundary

- *A priori* analysis show how the value of Smagorinsky coefficient should change as a function of these local parameters

- The functional description of the joint dependences are not amenable to factorization

- *A priori* analysis of neutrally buoyant isotropic turbulence DNS data show that enforcing the Germano identity in a conditionally average sense and solving the resulting equation iteratively recovers the measured trends

- The next step is to implement the suggested model and test its performance in *a posteriori* tests.