NCAR TOY Workshop
Geophysical Turbulence Phenomena
Turbulence Theory and Modeling
29 February 2008

Requirements to Predict the Surface Layer with High Accuracy at High Reynolds Numbers using Large-eddy Simulation*

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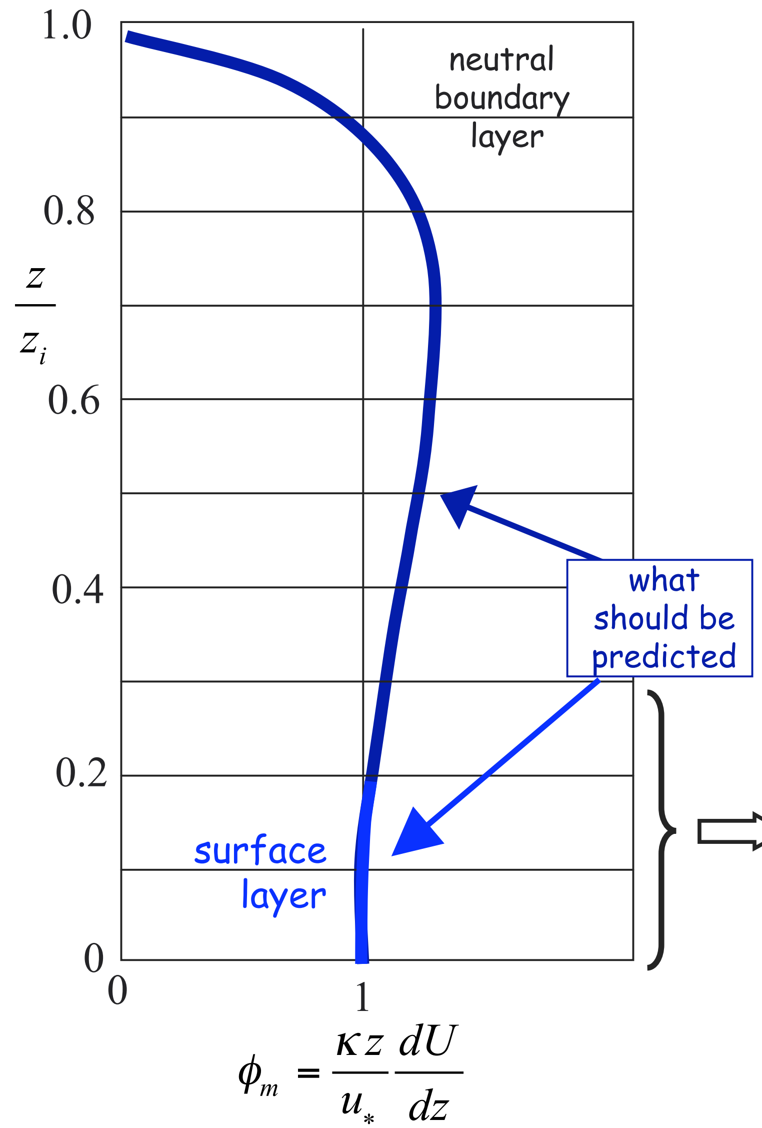
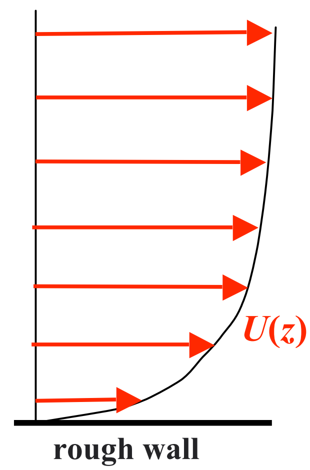
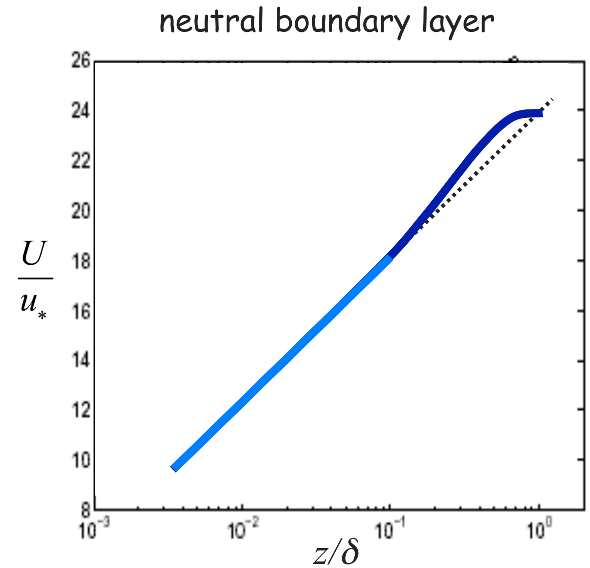
*supported by the Army Research Office

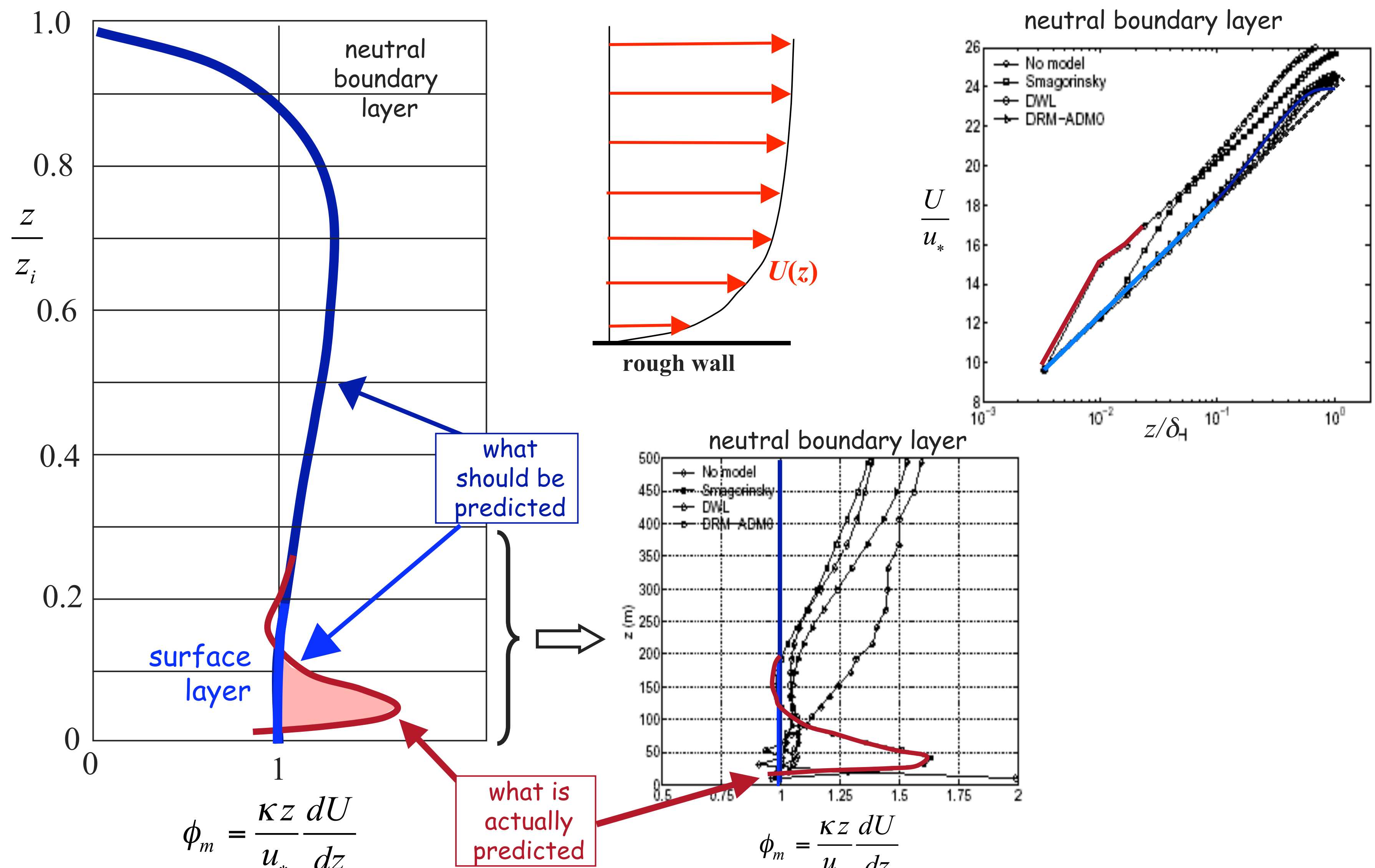
Fundamental Errors in LES Predictions in the Surface Layer of the Atmospheric Boundary Layer





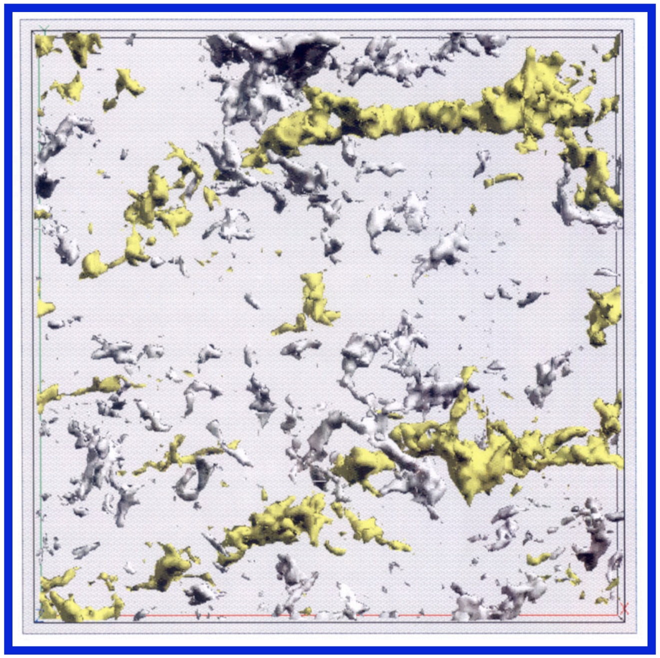


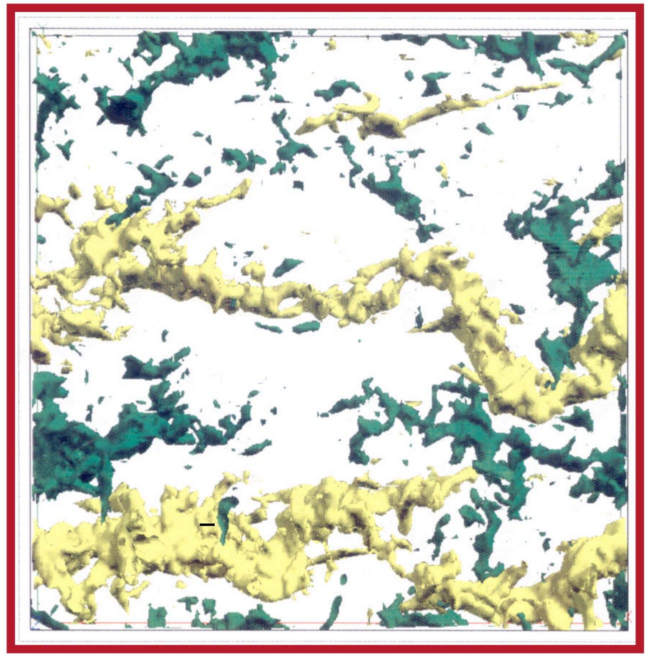
Fundamental Errors in LES Predictions in the Surface Layer of the Atmospheric Boundary Layer



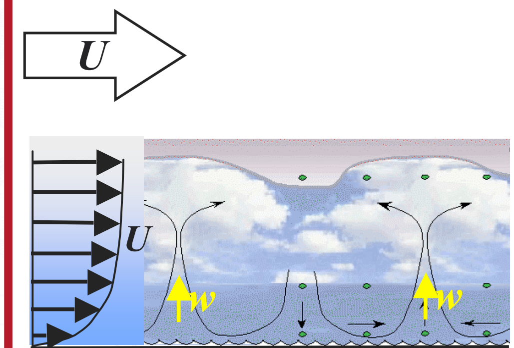
Chow, Street, Xue, Ferziger *JAS* 62, 2005

The Importance of the Overshoot





Moderately Convective Atmospheric Boundary Layer



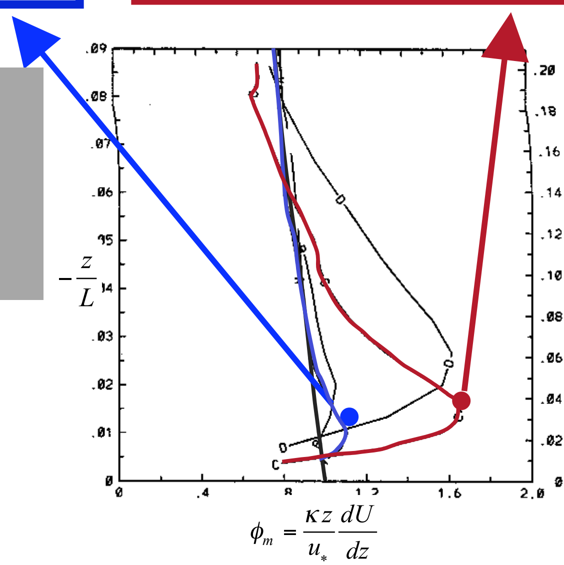
isosurfaces of vertical velocity:

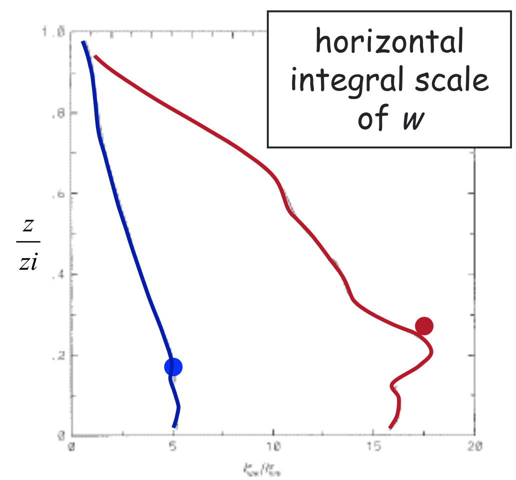
up: $w > 0$ (yellow)

down: $w < 0$ (white or green)

$$-\frac{z_i}{L} \approx 8$$

Khanna & Brasseur 1998, JAS 55

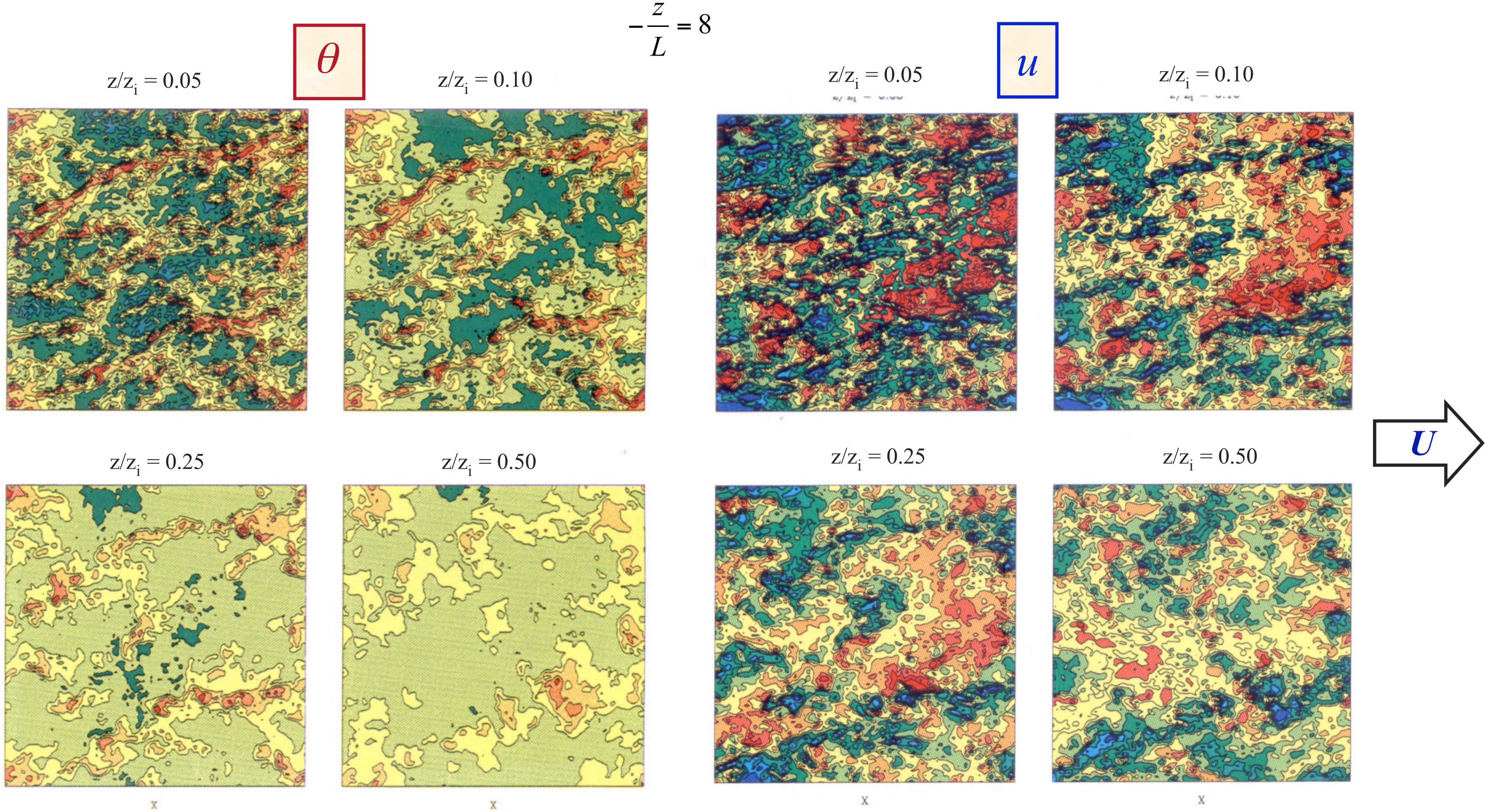




Why the Overshoot Alters Turbulence Structure

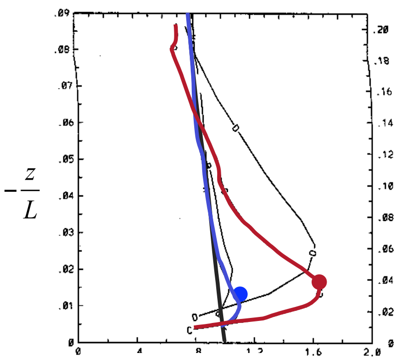
Moderately Convective ABL

$$-\frac{z}{L} = 8$$

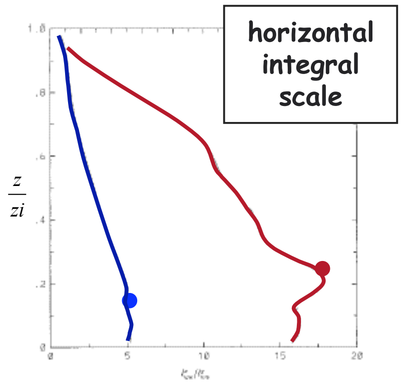


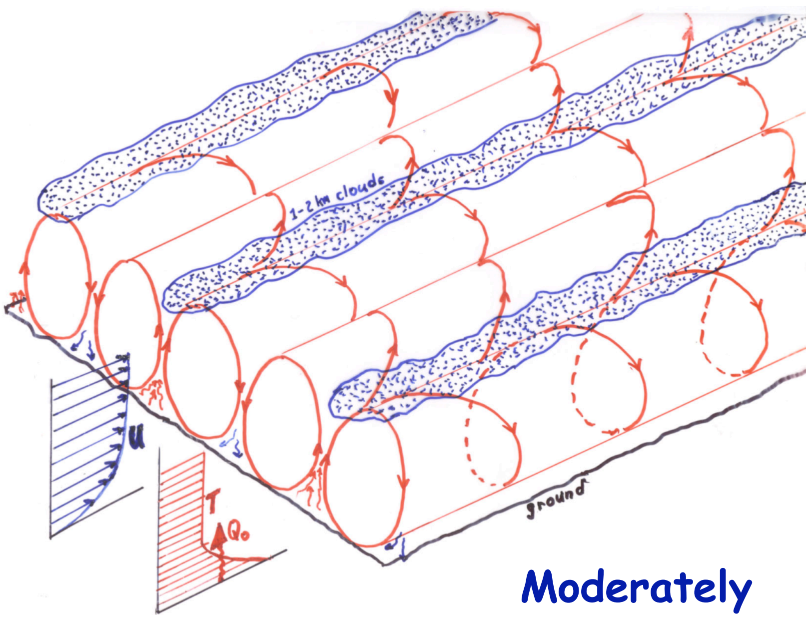
Khanna & Brasseur 1998, JAS 55

Consequences of the Overshoot



$$\phi_m = \frac{\kappa z}{u_*}\frac{dU}{dz}$$





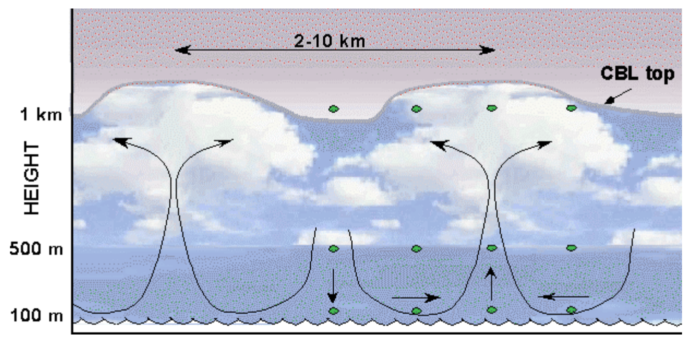
Moderately Convective ABL

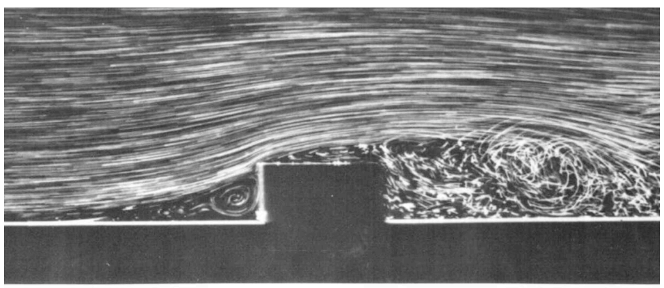
Over-prediction of mean shear in the surface layer produces poor predictions throughout the ABL of:

- turbulence production
- thermal eddying structure (e.g., rolls)
- vertical transport, dispersion and eddy structure of momentum, temperature, humidity, contaminants, toxins, …
- correlations, turbulent kinetic energies,…
- cloud cover, CO_2 transport, radiation, …

16-year History of the Overshoot

Relevant to any LES of boundary layers where the viscous sublayer is unresolved or nonexistent.
… enhanced with direct exchange between inner and outer boundary layer:

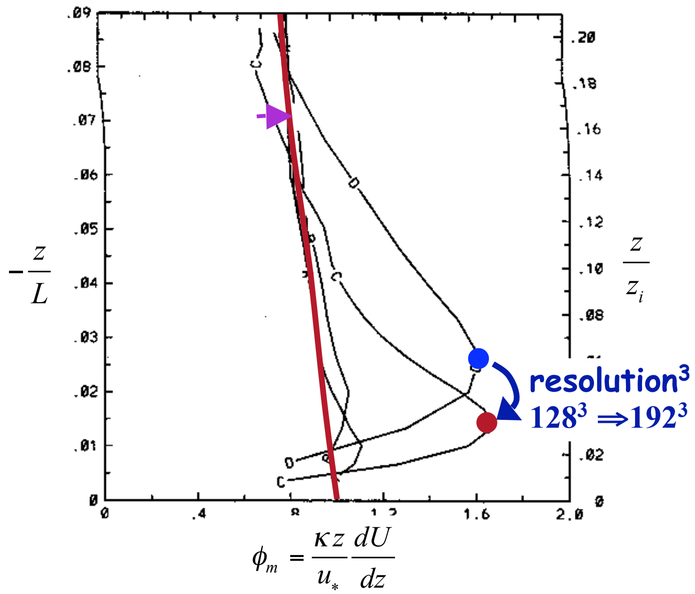




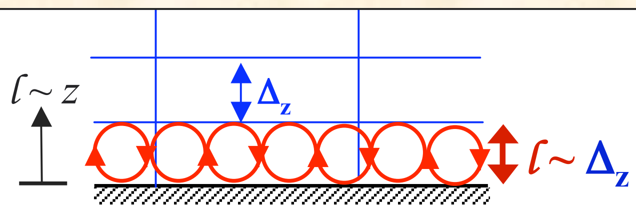
1. **Mason & Thomson 1992, *JFM* 242.**
2. Sullivan, McWilliams & Moeng 1994, *BLM* 71.
3. Andren, Brown, Graf, Mason, Moeng, Nieuwstadt & Schumann 1994 *QJR Meteor Soc* 120 (comparison of 4 codes: Mason, Moeng, Neiustadt, Schumann).
4. Khanna & Brasseur 1997, *JFM* 345.
5. Kosovic 1997, *JFM* 336.
6. Khanna & Brasseur 1998, *JAS* 55.
7. Juneja & Brasseur 1999 *Phys Fluids* 11.
8. Port-Agel, Meneveau & Parlange 2000, *JFM* 415.
9. Zhou, Brasseur & Juneja 2001 *Phys Fluids* 13.
10. Ding, Arya, Li 2001, *Environ Fluid Mech* 1.
11. Reselsperger, Mahé & Carlotti 2001, *BLM* 101.
12. Esau 2004 *Environ Fluid Mech* 4.
13. Chow, Street, Xue & Ferziger 2005, *JAS* 62
14. Anderson, Basu & Letchford 2007, *Environ Fluid Mech* 7.
15. Drobinski, Carlotti, Redelsperger, Banta, Masson & Newson 2007, *JAS* 64.
16. Moeng, Dudhia, Klemp & Sullivan 2007 Monthly Weather Rev 135.

Clues from Previous Studies

1. The overshoot is tied to the grid



2. Inherent under-resolution at the first grid level

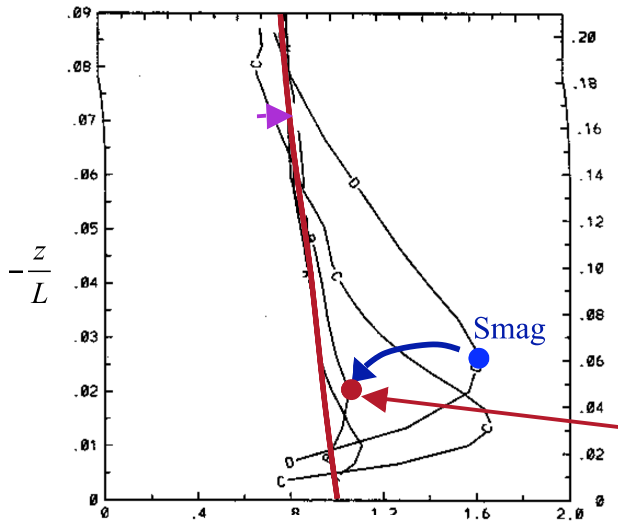


Juneja & Brasseur 1999, Phys. Fluids 11

Khanna & Brasseur 1997, *JFM* 345

Clues

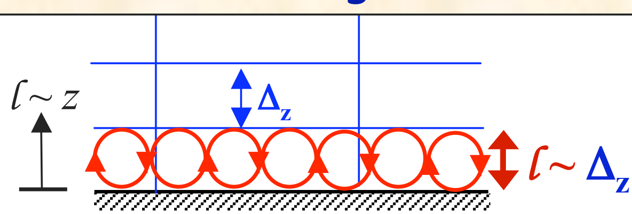
1. The overshoot is tied to the grid



$$\phi_m = \frac{\kappa z}{u_*}\frac{dU}{dz}$$

Sullivan, McWilliams & Moeng 1994, *BLM* 71

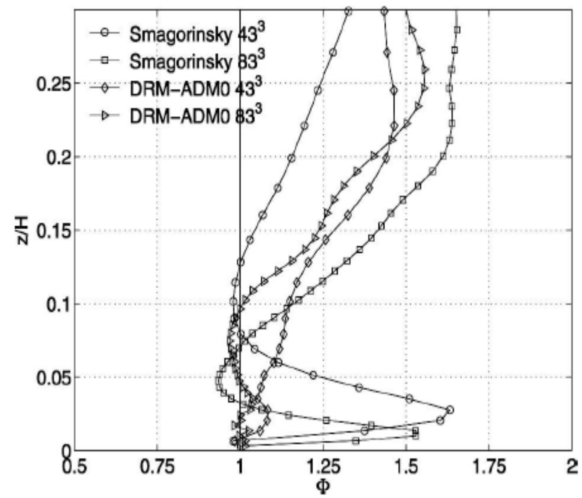
2. Inherent under-resolution at the first grid level



Juneja & Brasseur 1999, Phys. Fluids 11

Khanna & Brasseur 1997, JFM 345

3. The overshoot is sensitive to the SFS model



Chow, Street, Xue & Ferziger 2005, JAS 62

4. Lack of grid independence

⇒ not strictly a modeling issue.

Into the Future

1. **Mason & Thomson 1992,**
2. Sullivan, McWilliams & M
3. Andren, Brown, Graf, Mas
   120 (comparison of 4 codes
4. Khanna & Brasseur 1997, *J*
5. Kosovic 1997, *JFM* 336.
6. Khann
7. Juneja
8. Port-A
9. Zhou,
10. Ding,
11. Resels
12. Esau 2
13. Chow
14. Ander
15. Drobi
16. Moen

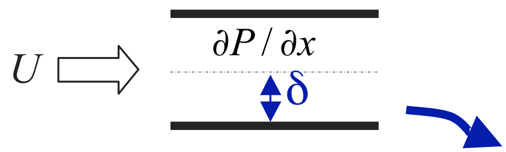
What is known after 15 years:

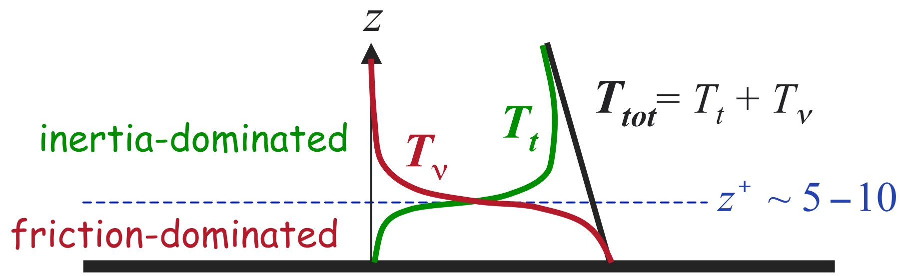
- The overshoot is fundamental to LES of shear-dominated surface layers.
- The overshoot is somehow connected to the grid
- connected

Today's Discussion:

- We have (finally) found the source(s) of the overshoot and its consequences.
- The solution is a framework in which high-accuracy LES can be developed.
- The framework involves and interplay between: (1) grid resolution,
  (2) SFS model,
  (3) numerical algorithm,
  (4) grid aspect ratio.

The First Discovery: Scaling
Mean Smooth-Wall Channel Flow





stationary, fully developed, mean:

$$\frac{\partial P}{\partial x} = \frac{\rho u_*^2}{\delta} = \frac{\partial T_{tot}}{\partial z} = \frac{\partial T_t}{\partial z} + \frac{\partial T_\nu}{\partial z}$$

$$\Rightarrow \quad \mu \frac{\partial S}{\partial z} = \frac{\rho u_*^2}{\delta} - \frac{\partial T_t}{\partial z}$$

$$T_\nu = \mu \frac{\partial U}{\partial z} \equiv \mu S(z)$$

$$T_t \equiv -\rho \langle u'w' \rangle$$

$$T_t^+ \equiv \frac{T_t}{\rho u_*^2}$$

$$z^+ \equiv \frac{z}{\ell_\nu}$$

$$\ell_\nu = \nu / u_*$$

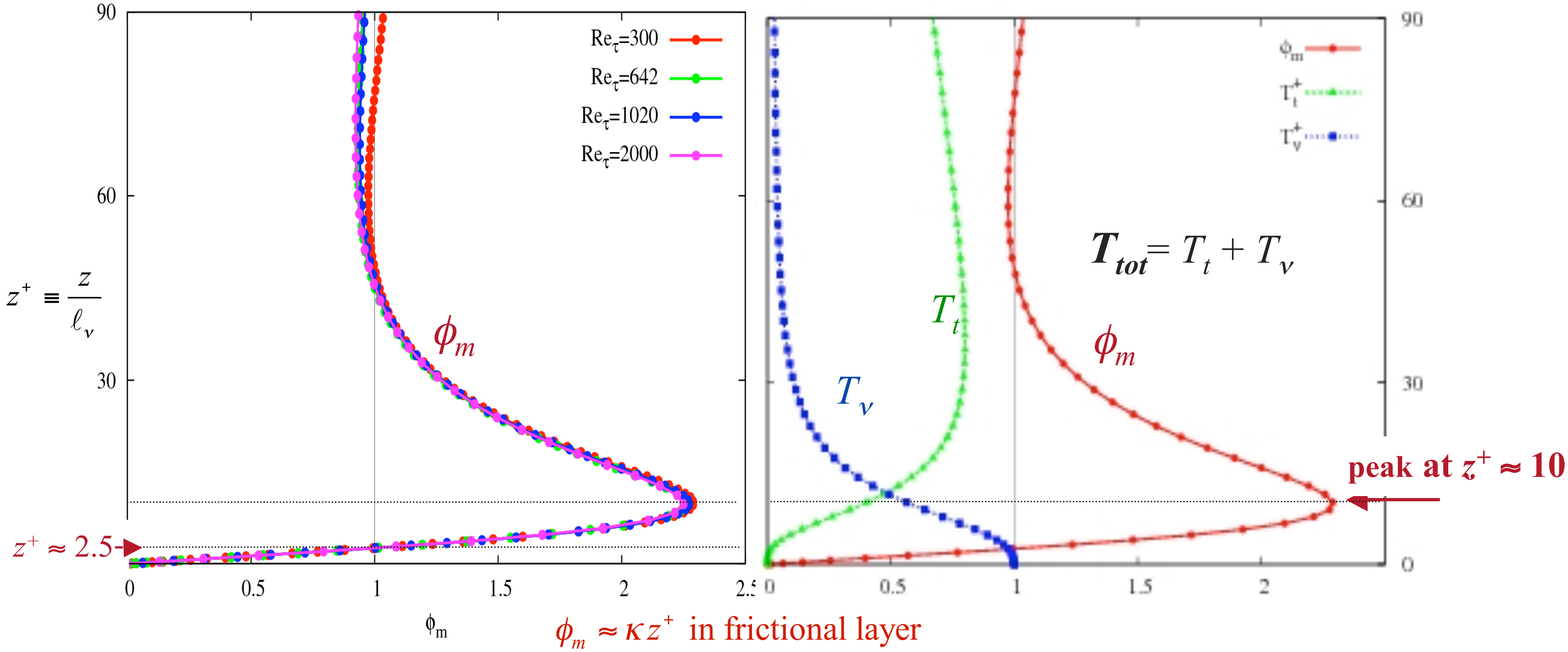
inertial scaling: $\phi_m = \frac{\kappa z}{u_*} S \quad \Rightarrow \quad \frac{T_\nu}{\rho u_*^2} = \left(\frac{\nu}{\kappa u_*^2} \right) \phi_m$

integrate $0 \to z$: $\phi_m = \kappa z^+ \left(1 - T_t^+ - \frac{z}{\delta} \right) \approx \kappa z^+$ in friction-dominated layer

$\kappa \approx 0.4 \;\; \Rightarrow \;\; \phi_m$ exceeds 1 when $z^+ > 2.5$ (!)

Smooth-Wall Channel Flow

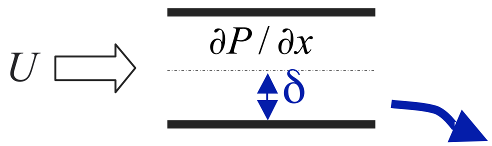
DNS data from Iwamoto et al., Jimenez et al..



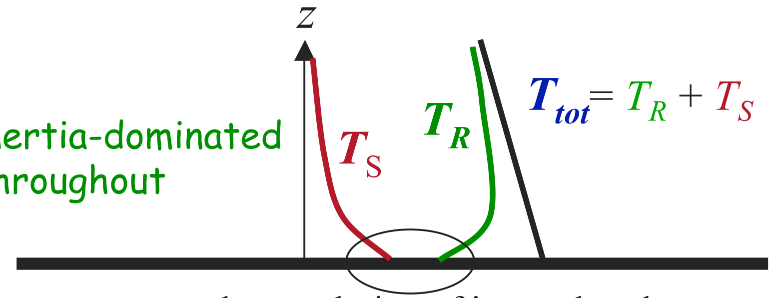
Conclusions

1. In the smooth-wall channel flow the overshoot in ϕ_m is real.
2. The real overshoot in ϕ_m arises from applying inertial scale *z* in a frictional layer that has characteristic viscous scale $\ell_\nu = \nu / u_*$

The First Discovery: Scaling
Mean LES of high Re or Rough-Wall Channel Flow



inertia-dominated throughout



under-resolution of integral scales at first few grid levels

$$\frac{\partial u_i^r}{\partial t} + \frac{\partial \widehat{(u_i^r u_j^r)}^r}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \hat{p}^r}{\partial x_i} + \frac{\partial \tau_{ij}^{SFS}}{\partial x_j}$$

$$T_R \equiv -\rho\left\langle u^{r\prime} w^{r\prime}\right\rangle$$

$$T_S = -\rho\left\langle \tau_{13}^{SFS}\right\rangle$$

stationary, fully developed, mean:

$$\frac{\partial P}{\partial x} = \frac{\rho u_*^2}{\delta} = \frac{\partial T_{tot}}{\partial z} = \frac{\partial T_R}{\partial z} + \frac{\partial T_S}{\partial z}$$

Extract Viscous Content of SGS Model:

define "LES viscosity" for strong shear flow

$$\nu_{les}(z) \equiv \frac{T_S(z)}{2\left\langle S_{13}^r\right\rangle}, \quad \nu_{LES} \equiv \nu_{les}(z_1)$$

IF $\tau_{ij}^{SFS} \equiv -2\nu_t S_{ij}^r$,

we find $\nu_{LES} \approx \langle \nu_t \rangle_1$

$$T_R^+ \equiv \frac{T_R}{\rho u_*^2}$$

$$z_{LES}^+ \equiv \frac{z}{\nu_{LES} / u_*}$$

$$\tilde{\nu}_{les} \equiv \frac{\nu_{les}(z)}{\nu_{LES}}$$

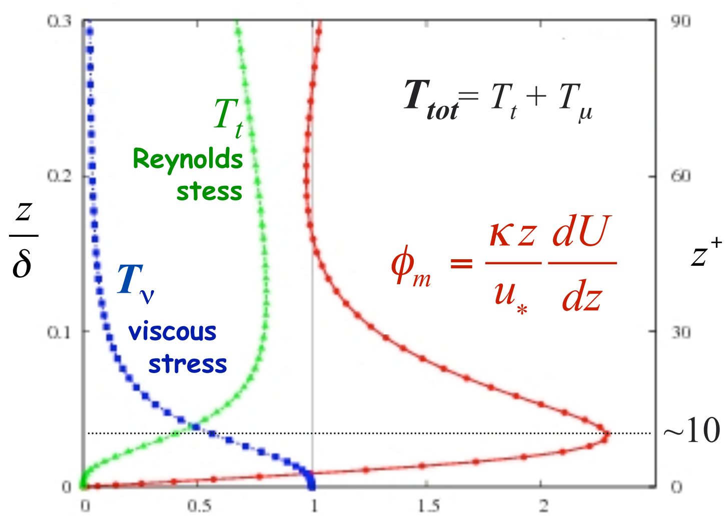
Inertial Scaling

… integrate 0 → z:

$$\phi_m = \frac{\kappa z_{LES}^+}{\tilde{\nu}_{les}(z)}\left(1 - T_R^+ - \frac{z}{\delta}\right) \approx \kappa z_{LES}^+ \left(1 - T_R^+\right) \text{ near the surface}$$

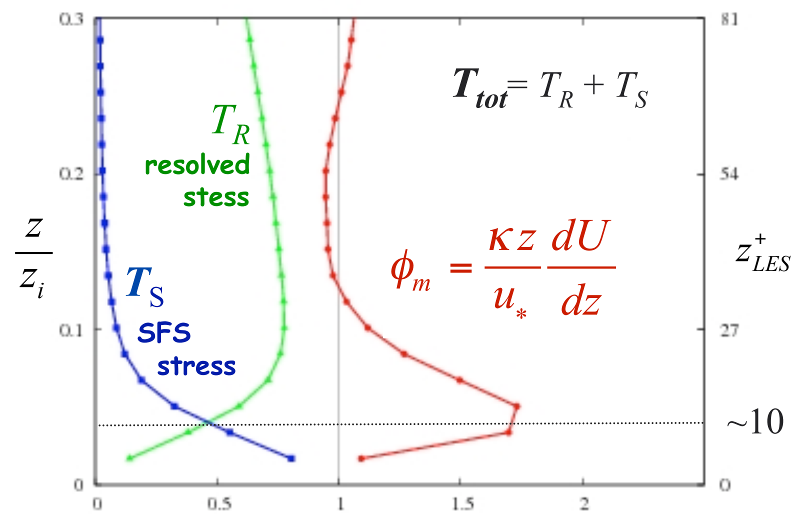
The First Discovery:
A Spurious Frictional Surface Layer

DNS: Smooth-wall Channel Flow



$\phi_m \approx \kappa z^+ =$ in friction-dominated layer

LES: Rough-wall ABL



$\phi_m \approx \kappa z^+_{LES} =$ near the first grid level

$z^+ = \frac{z}{\nu / u_*}$ where ν parameterizes real friction

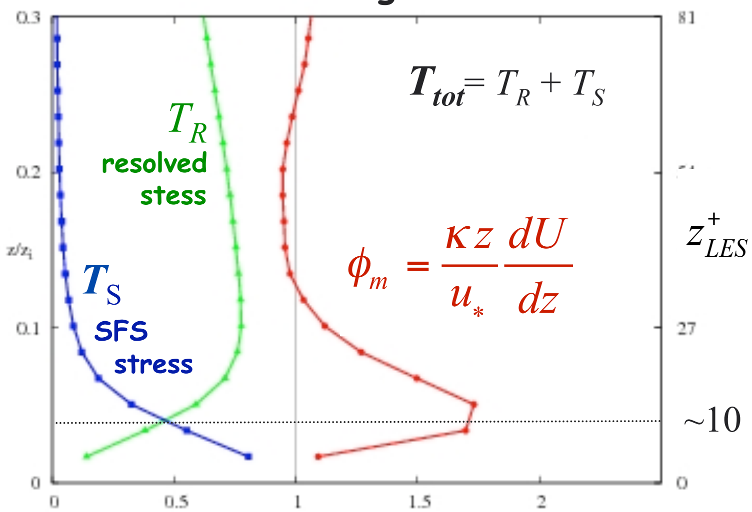
$z^+_{LES} = \frac{z}{\nu_{LES} / u_*}$ where ν_{LES} parameterizes friction in the (inertial) SFS stress

Conclusion

The overshoot in ϕ_m arises from applying an inertial scaling to a numerical LES "viscous" layer

The First Discovery:
A Requirement to Eliminate the Overshoot

LES of the Rough-wall ABL



$$z^+_{LES} = \frac{z}{\ell_{\nu_{LES}}}$$

a numerical LES "viscous" scale

$$\ell_{\nu_{LES}} \equiv \frac{\nu_{LES}}{u_*}$$

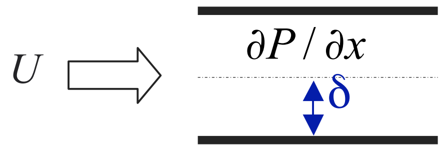
ν_{LES} is a "numerical-LES viscosity"

The overshoot arises from "numerical-LES friction" at the surface akin to the real frictional layer on smooth walls

$$\Re \equiv \left(\frac{T_R}{T_S}\right)_{z_1} > \Re^* \sim O(1)$$

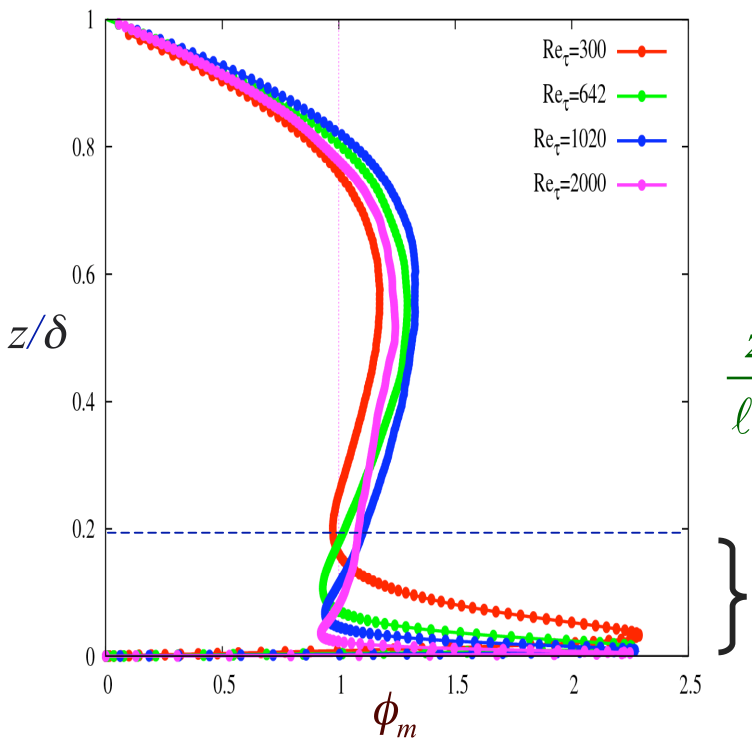
⇒ To eliminate the overshoot the ratio T_R/T_S must exceed a critical value ~ O(1) at the first grid level.

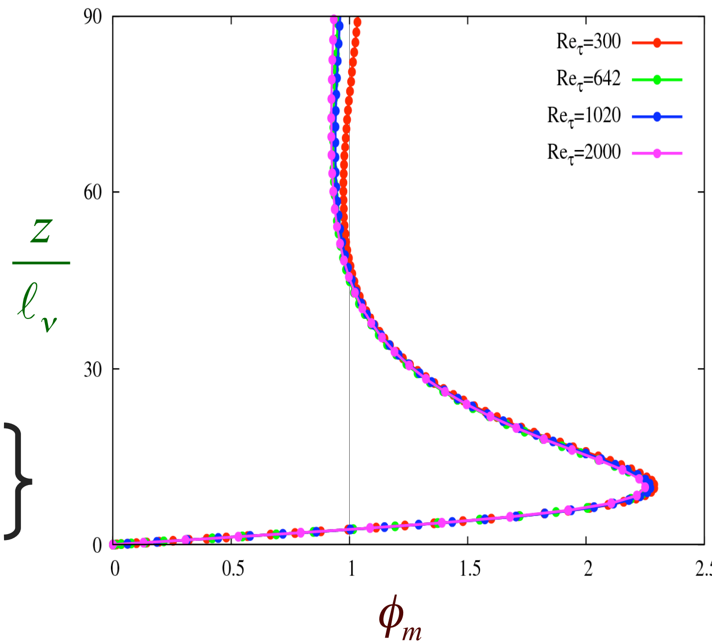
The Second Discovery: Relative Inertia to Friction in the Real BL



$$\mathrm{Re}_\tau \equiv \frac{u_* \delta}{\nu} = \frac{\delta}{\ell_\nu}, \quad \text{where } \ell_\nu = \nu / u_*$$

$\Rightarrow \mathrm{Re}_\tau > \mathrm{Re}_\tau^*$ to support an inertial surface layer





DNS data from Iwamoto et al., Jimenez et al..

The Second Discovery: Relative Inertia to LES Friction in the Simulation

define $\mathrm{Re}_{LES} \equiv \dfrac{u_* \delta}{\nu_{LES}} = \dfrac{\delta}{\ell_{\nu_{LES}}}$ LES Reynolds Number

$\ell_{\nu_{LES}} = \nu_{LES} / u_*$ $\Rightarrow \mathrm{Re}_{LES} > \mathrm{Re}^*_{LES}$ to support an inertial surface layer

Scaling $\tau_{ij}^{SFS} \equiv -2\nu_t S_{ij}^r, \quad \nu_t = (C_s \Delta)^2 \, | S |$

Smag model: $\nu_{LES} \approx \langle \nu_t \rangle |_1 \approx 2^{-1/2} (C_s \Delta)^2 \left. \dfrac{\partial U}{\partial z} \right|_1 \approx 2^{-1/2} (C_s \Delta)^2 \dfrac{u_*}{\tilde{\kappa}_1} \dfrac{1}{\Delta_z}$

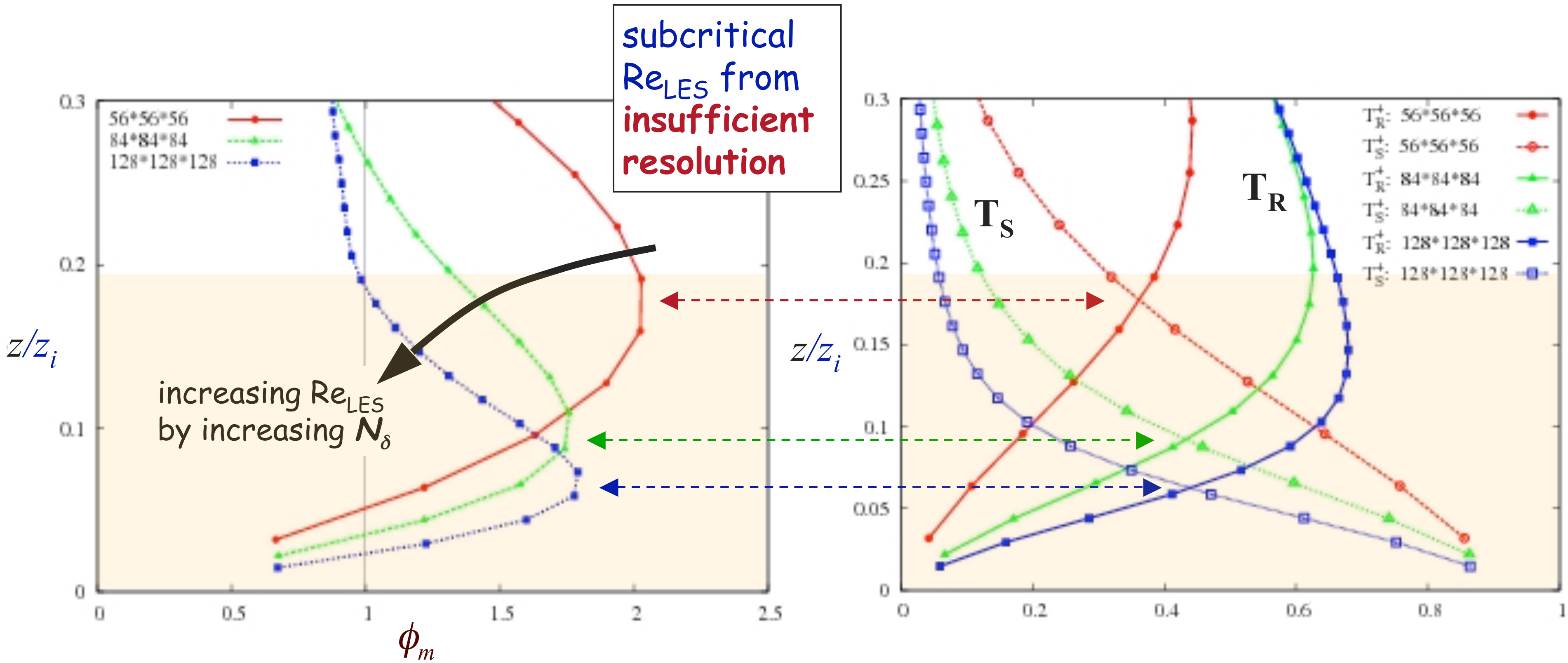
$\dfrac{\Delta}{\Delta_z} = (AR)^{2/3}$, where $AR \equiv \dfrac{\Delta_x}{\Delta_z} = \dfrac{\Delta_y}{\Delta_z} \Rightarrow$

$$\mathrm{Re}_{\mathrm{LES}} \approx \frac{\sqrt{2}\, \tilde{\kappa}_1 N_\delta}{C_S^2 (AR)^{4/3}}$$

$N_\delta \equiv \dfrac{\delta}{\Delta_z}$ $\Rightarrow$ resolution grid in vertical

$\Rightarrow \mathrm{Re}_{\mathrm{LES}} \propto N_\delta , \quad \mathrm{Re}_{\mathrm{LES}} \propto 1 / C_S^2 (AR)^{4/3}$

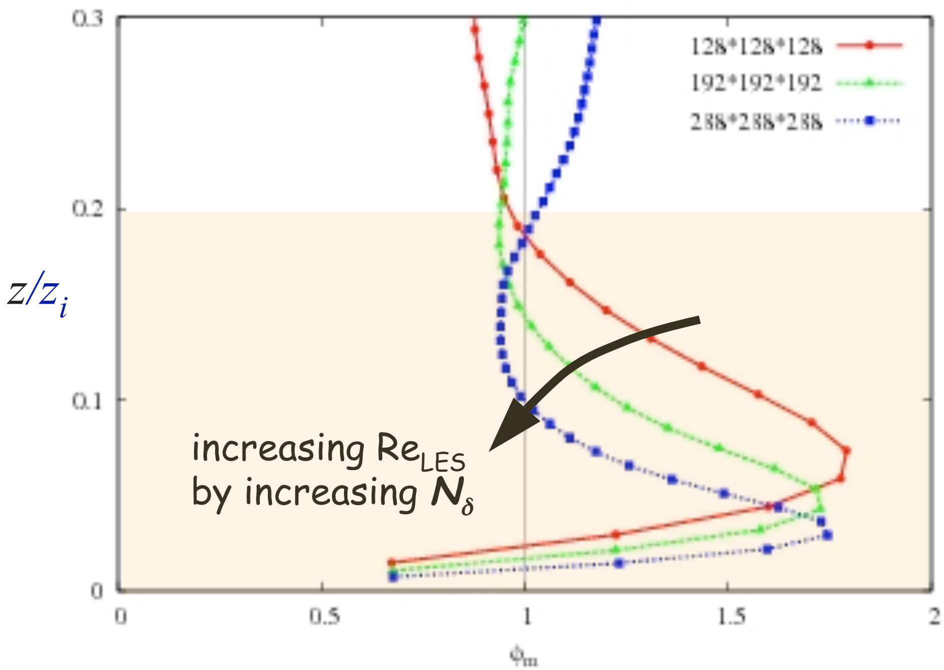
Numerical LES Viscous Effects at the Surface: Vertical Grid Resolution and T_R vs. T_S

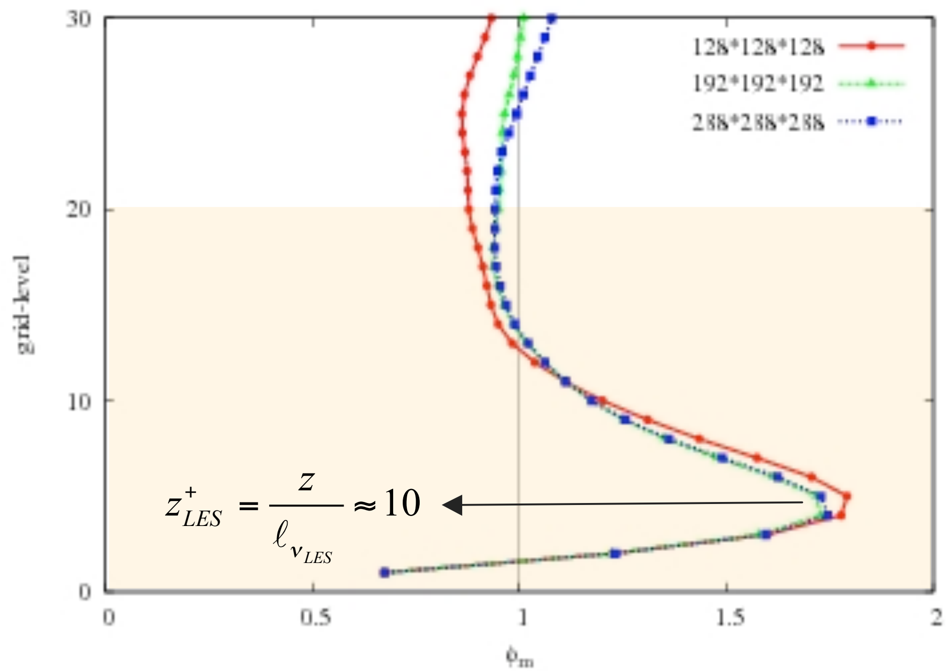


LES, Eddy Viscosity (Smag):

$$\mathrm{Re}_{\mathrm{LES}} \approx \frac{\sqrt{2}\;\tilde{\kappa}_1 N_\delta}{C_S^2 (AR)^{4/3}} \propto N_\delta$$

Why the Overshoot is Tied to the Grid





$$\ell_{\nu_{LES}} \equiv \frac{\nu_{LES}}{u_*} = \left(\frac{C_S^2 (AR)^{4/3}}{\sqrt{2}\;\tilde{\kappa}_1}\right)\Delta_z$$

$$\propto \Delta_z, \text{ fixed } C_S^2 (AR)^{4/3}$$

$\Rightarrow$ the overshoot cannot be "solved" with resolution

Putting the two Discoveries Together

1. For the simulation to have the possibility of producing a complete inertial surface layer, an LES Reynolds Number $\mathrm{Re}_{LES} \equiv \dfrac{u_* \delta}{\nu_{LES}} = \dfrac{\delta}{\ell_{\nu_{LES}}}$ must exceed a critical value, Re^*_{LES} requiring a minimum vertical resolution N^*_δ

2. To remove the overshoot in mean gradient, the resolved to SFS stress at the first grid level $\Re \equiv (T_R / T_S)_{z_1}$ must exceed a critical value $\Re^* \sim O(1)$

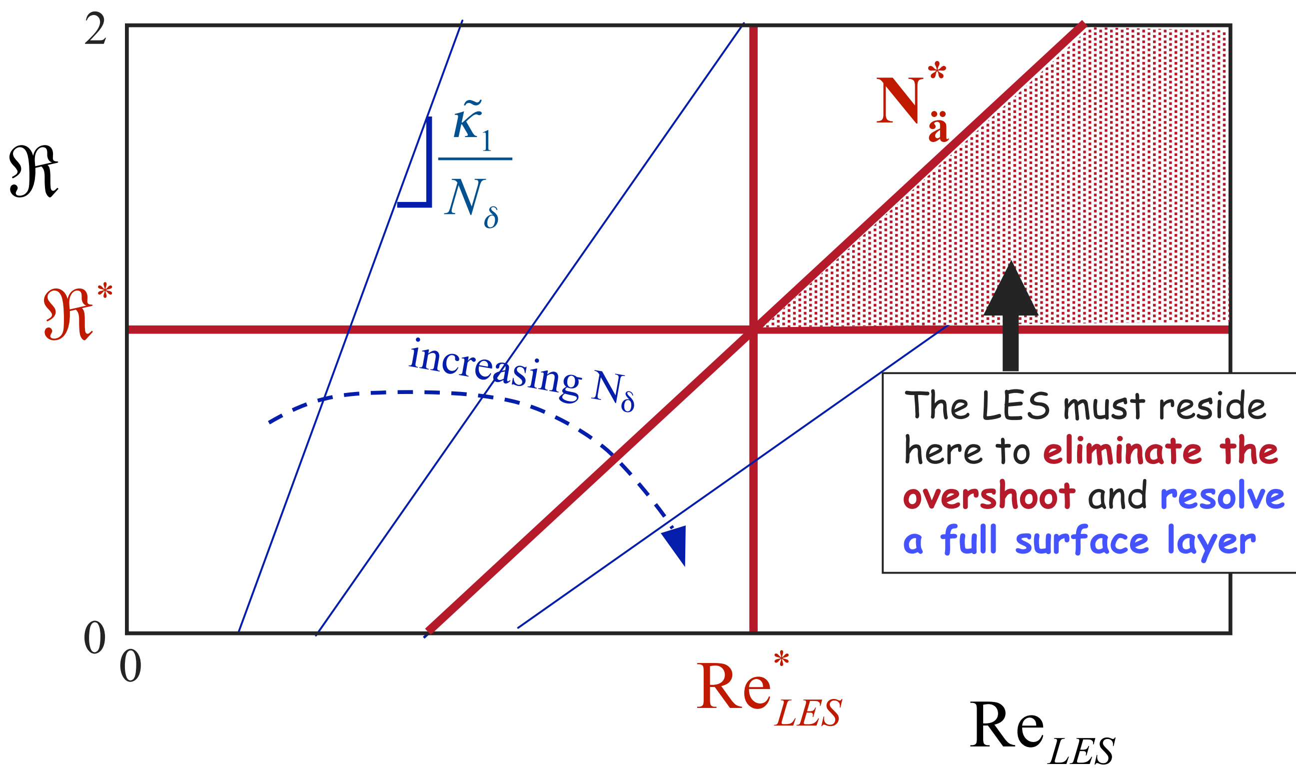
The Third Discovery

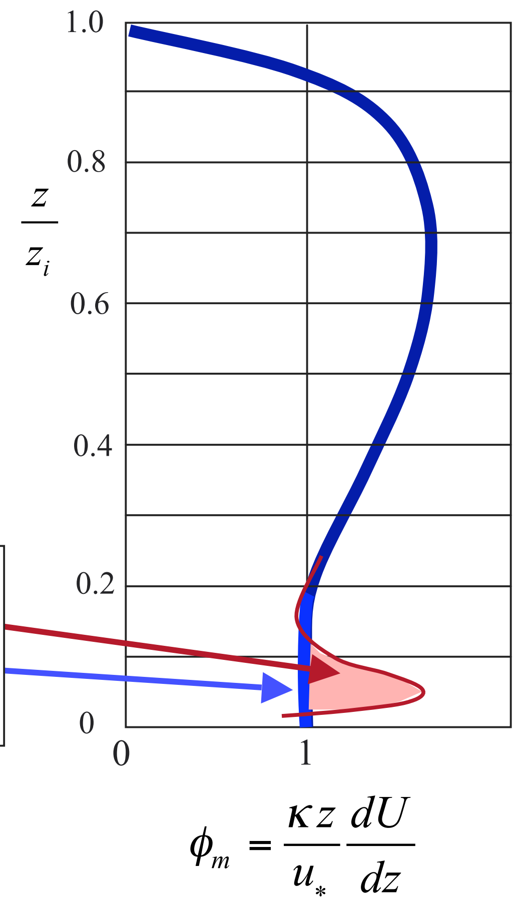
The $\Re - \mathrm{Re}_{LES}$ Parameter Space

In general,

$$\frac{T_R}{T_S} \equiv \Re = \left(\frac{\xi \tilde{\kappa}_1}{N_\delta} \right) \mathrm{Re}_{LES} - 1$$

$$\xi \approx \left(\frac{N_\delta - 1}{N_\delta} \right) \cos(\vec{S}_0, \hat{e}_x) \approx 0.9$$



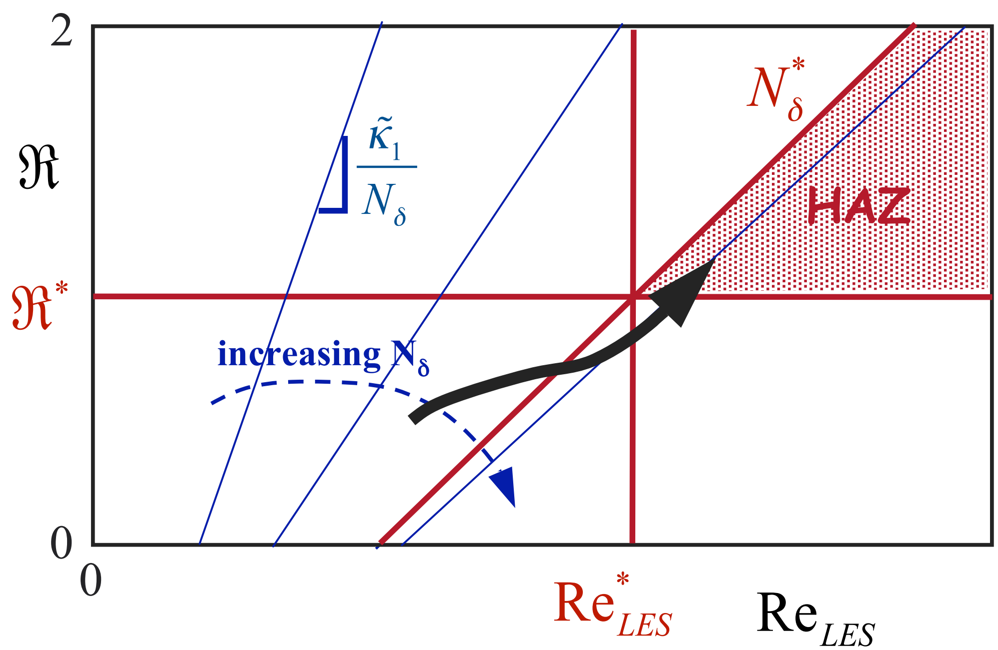


Designing High-Accuracy LES

In the $\Re - \mathrm{Re}_{LES}$ Parameter Space

For any SFS stress model:

$$\frac{\mathrm{T_R}}{\mathrm{T_S}} \equiv \Re = \left(\frac{\xi\tilde{\kappa}_1}{N_\delta}\right)\mathrm{Re}_{LES} - 1$$



Moving the simulation into the "High-Accuracy Zone (HAZ):

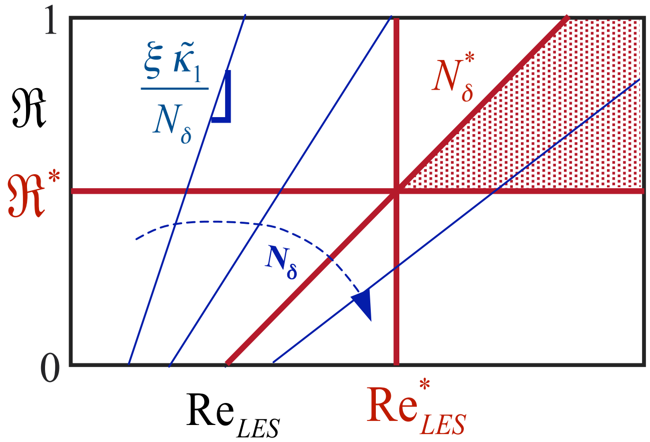
1. Adjust resolution in the vertical so that $N_\delta > N_\delta^*$
2. Adjust AR + model constant *together* until

$$\Re > \Re^* \text{ and } \mathrm{Re}_{LES} > \mathrm{Re}_{LES}^*$$

If using the Smagorinsky model:

$$\mathrm{Re}_{LES} = \sqrt{2}\tilde{\kappa}_1 \frac{N_\delta}{C_S^2 (AR)^{4/3}}$$

$$\Re = \frac{\sqrt{2}\xi\tilde{\kappa}_1^2}{C_S^2 (AR)^{4/3}} - 1$$

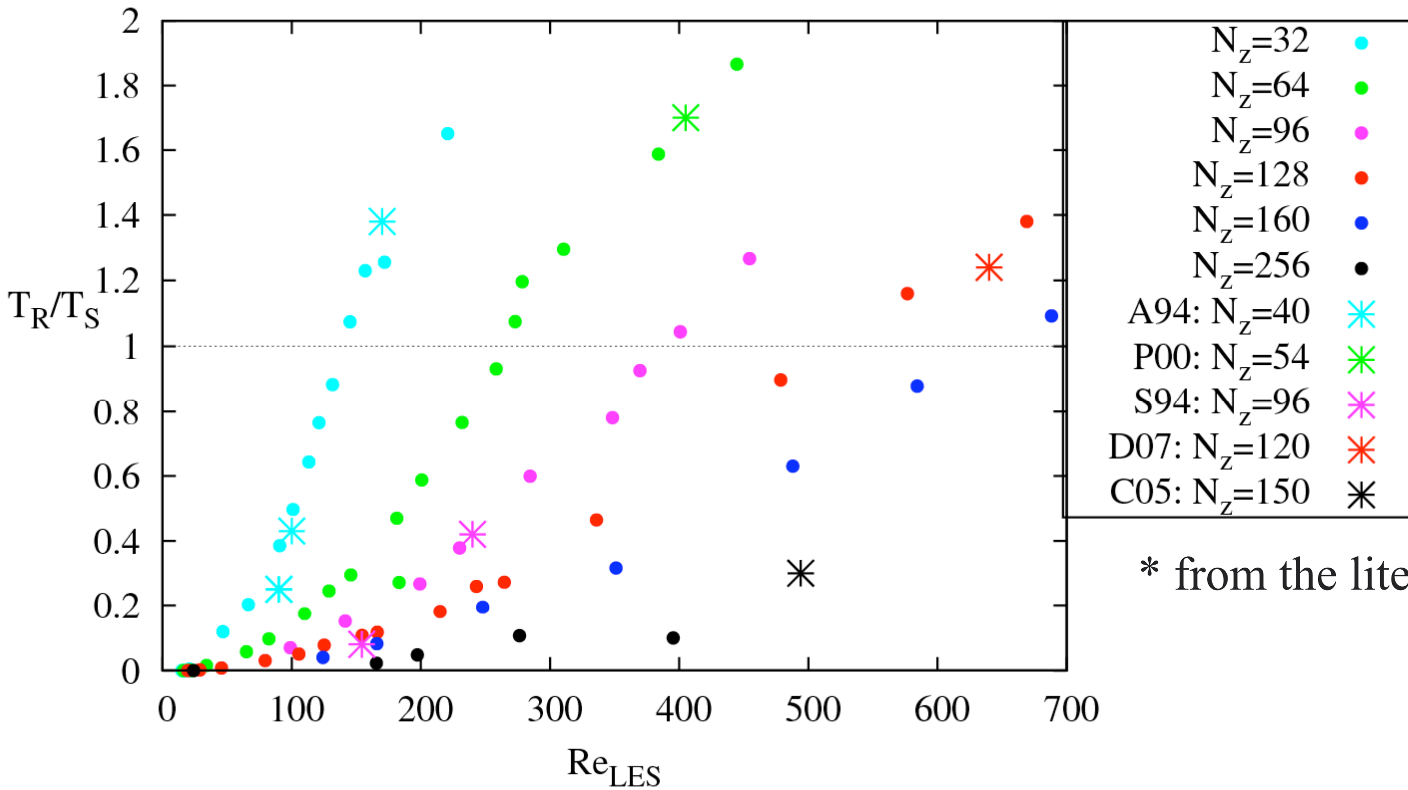


Numerical Experiments

$$\frac{T_R}{T_S} \equiv \Re = \left(\frac{\xi\tilde{\kappa}_1}{N_\delta}\right) Re_{LES} - 1$$

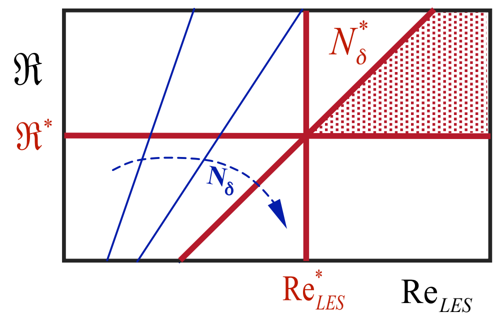
$$Re_{LES} = \sqrt{2}\tilde{\kappa}_1 \frac{N_\delta}{C_S^2 (AR)^{4/3}}$$

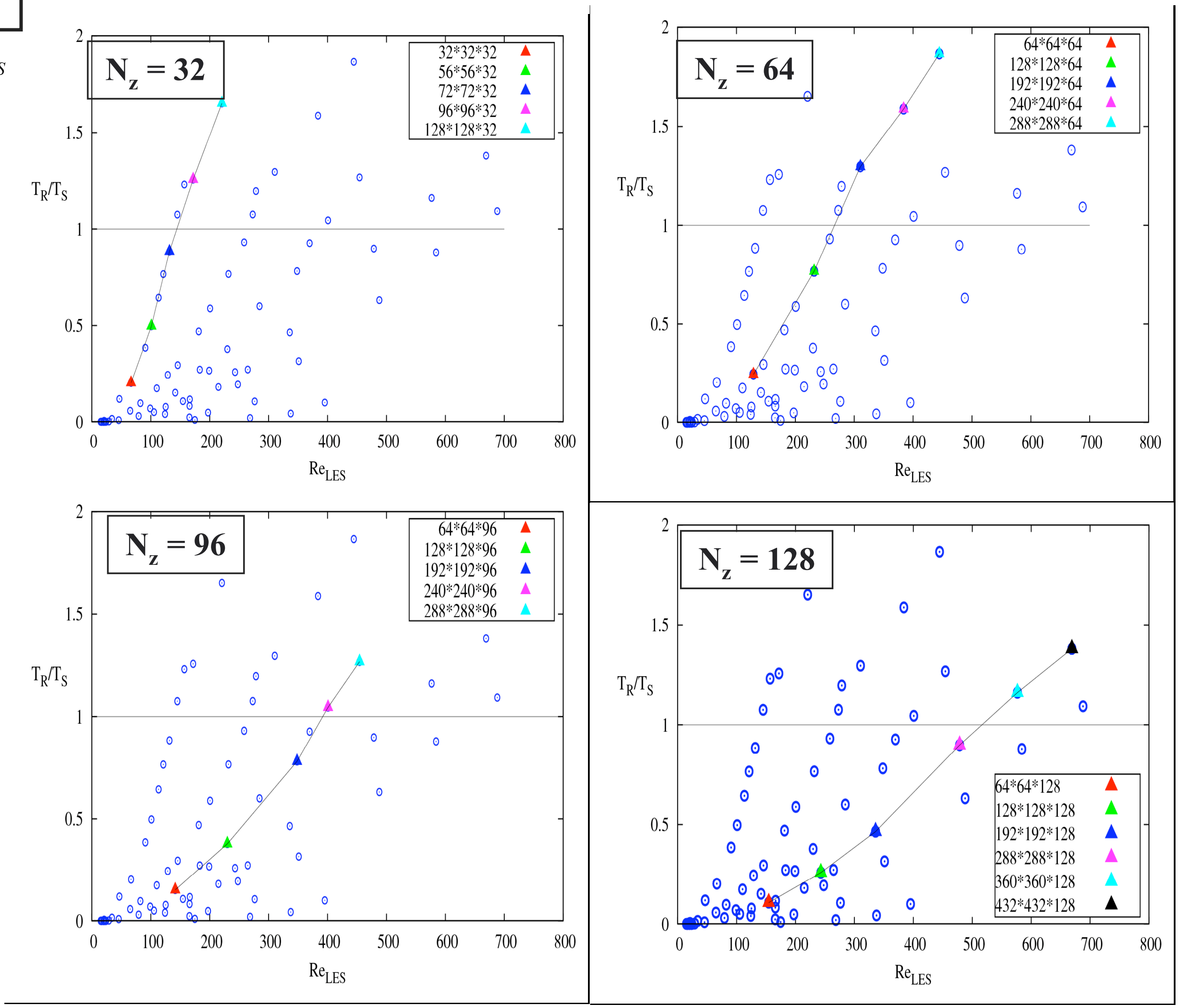
$$\Re = \frac{\sqrt{2}\xi\tilde{\kappa}_1^2}{C_S^2 (AR)^{4/3}} - 1$$

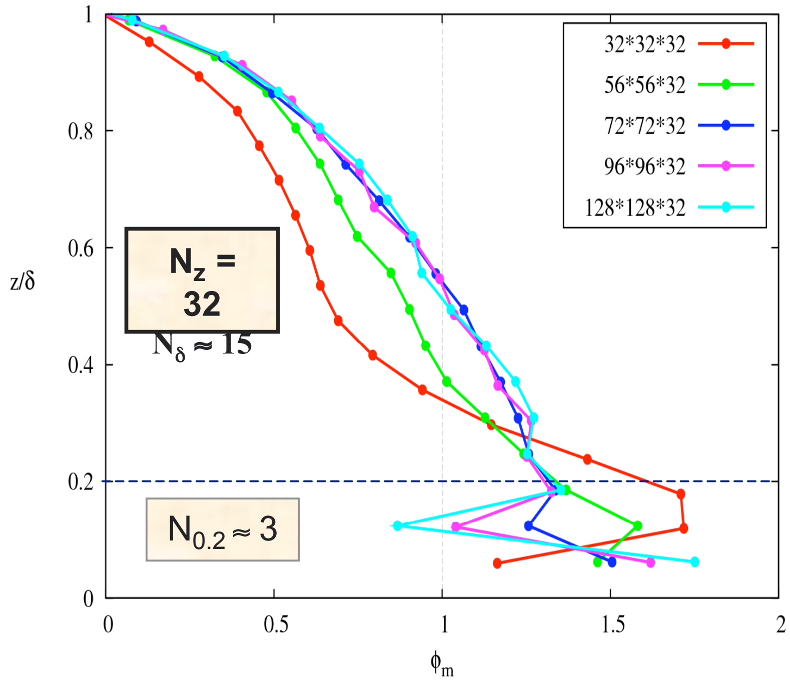


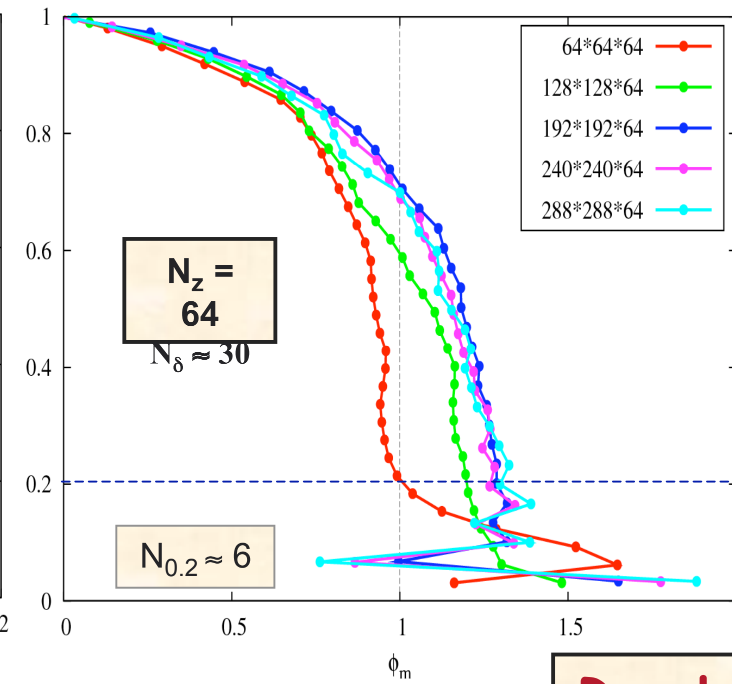
* from the literature

Numerical Experiments

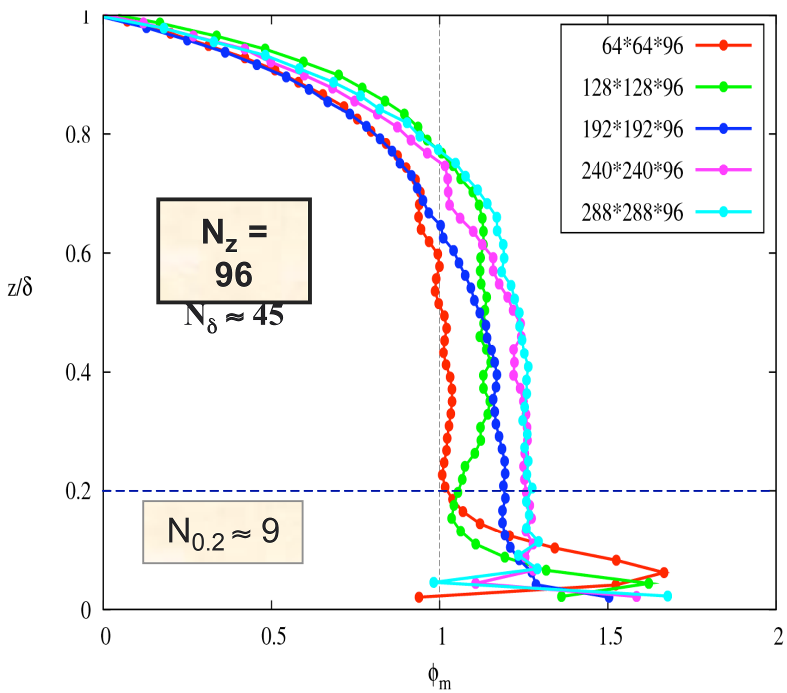


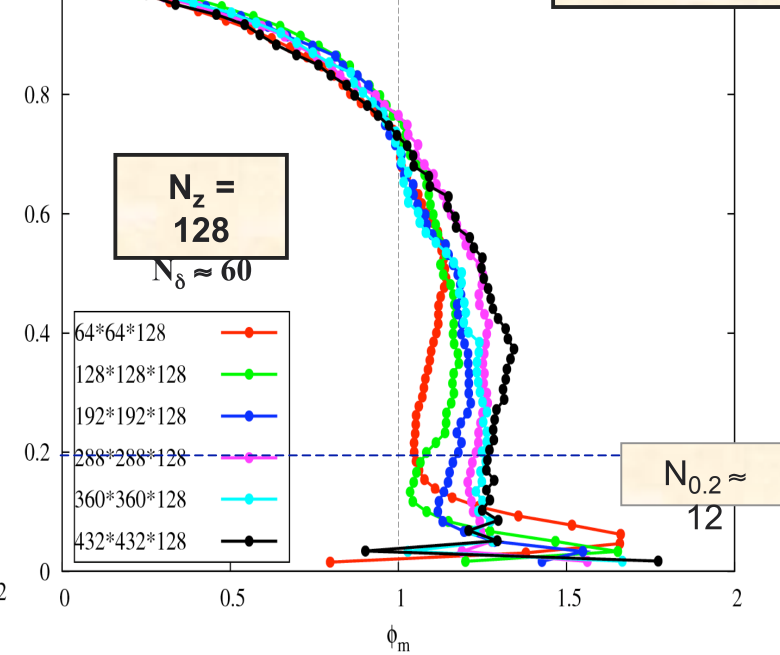


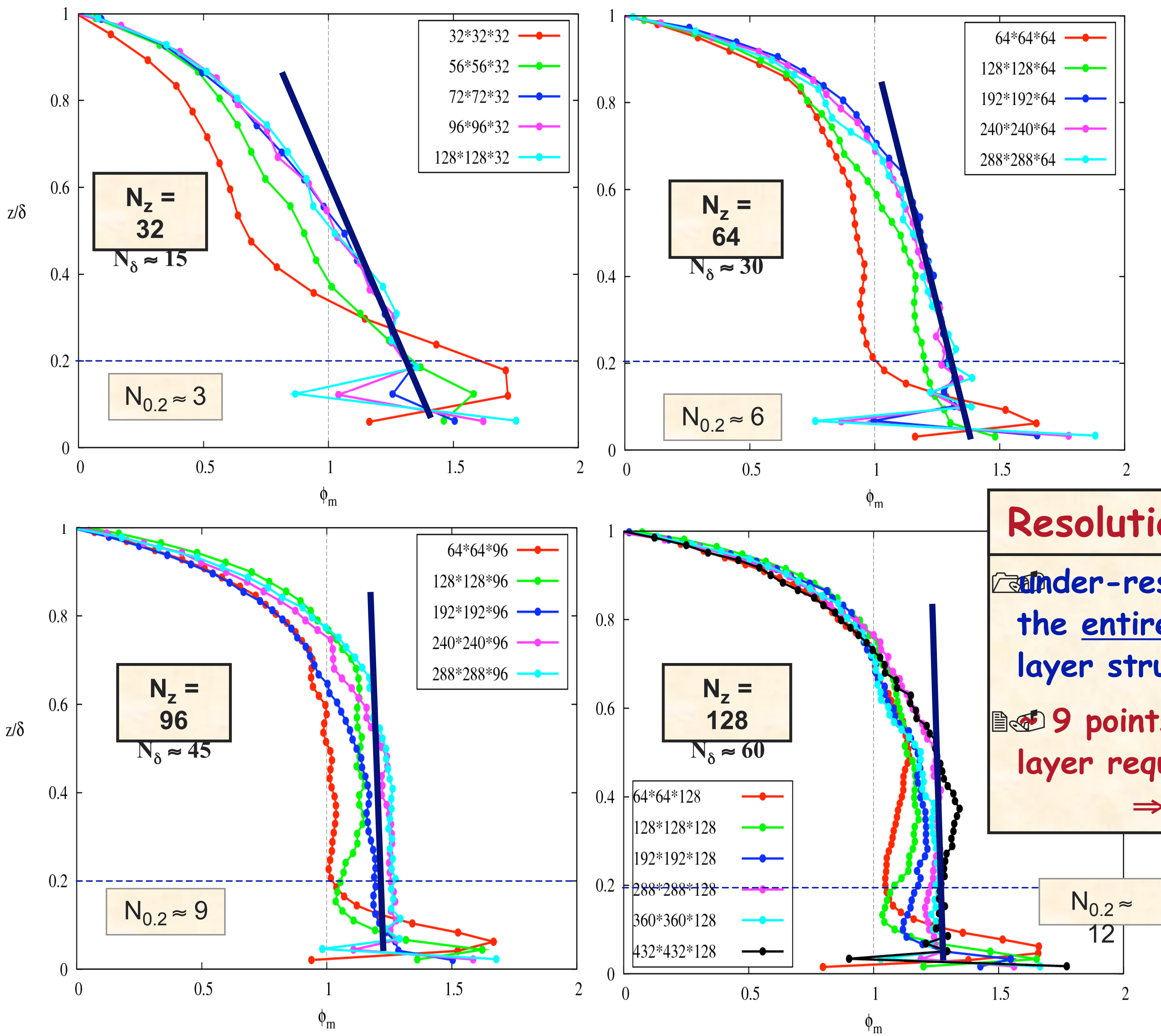




Resolution N_δ





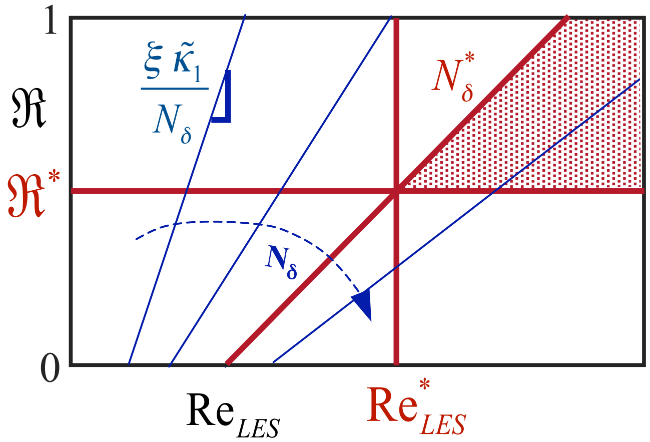


Resolution N_δ

- under-resolution alters the <u>entire</u> boundary layer structure
- 9 points in surface layer required

$\Rightarrow$ $N_\delta^* \approx 45$

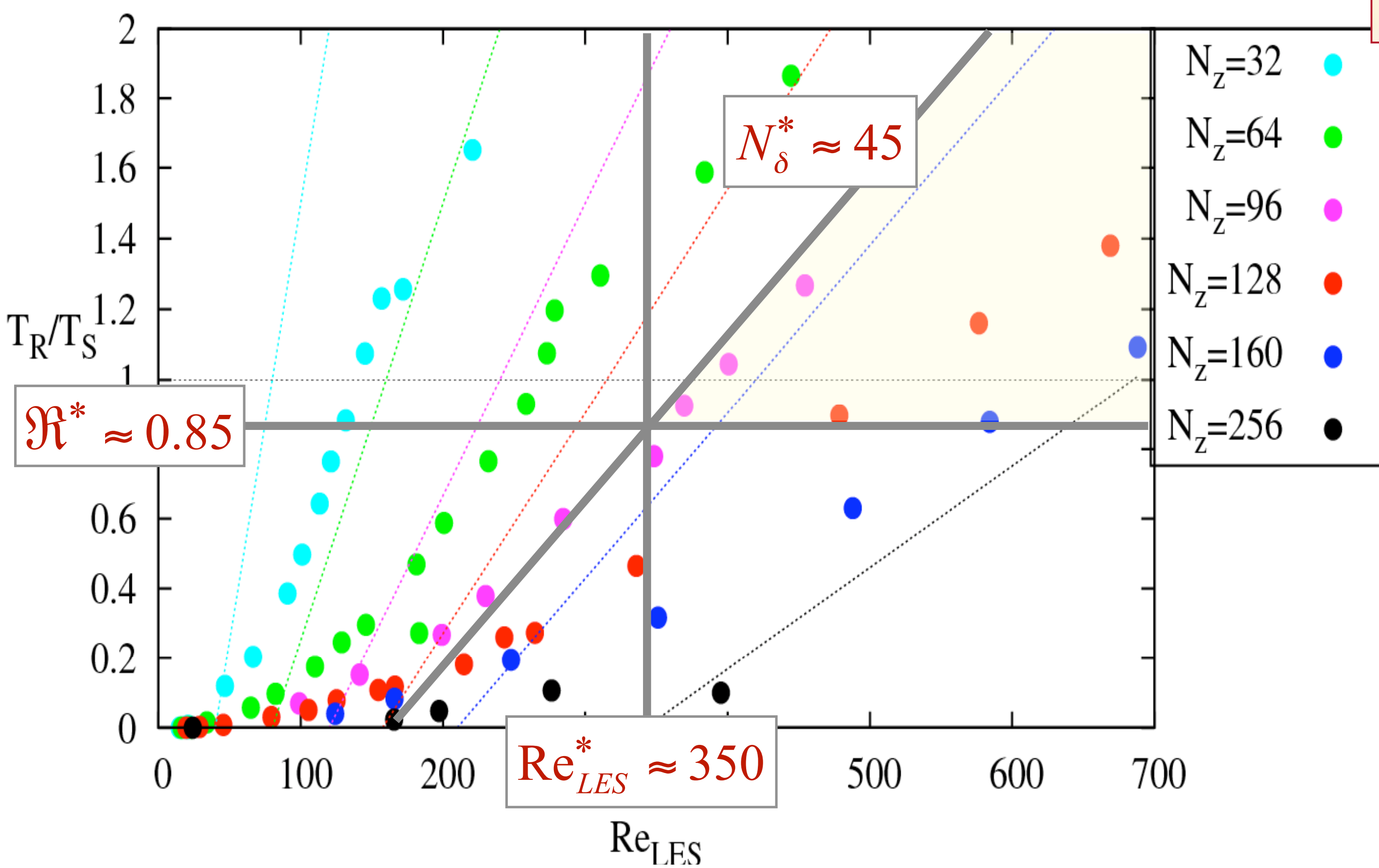
Numerical Experiments



$$\Rightarrow \frac{T_R}{T_S} \equiv \Re = \left(\frac{\xi\tilde{\kappa}_1}{N_\delta}\right) Re_{LES} - 1$$

$$Re_{LES} = \sqrt{2}\,\tilde{\kappa}_1 \frac{N_\delta}{C_S^2 (AR)^{4/3}}$$

$$\Re = \frac{\sqrt{2}\,\xi\tilde{\kappa}_1^2}{C_S^2 (AR)^{4/3}} - 1$$



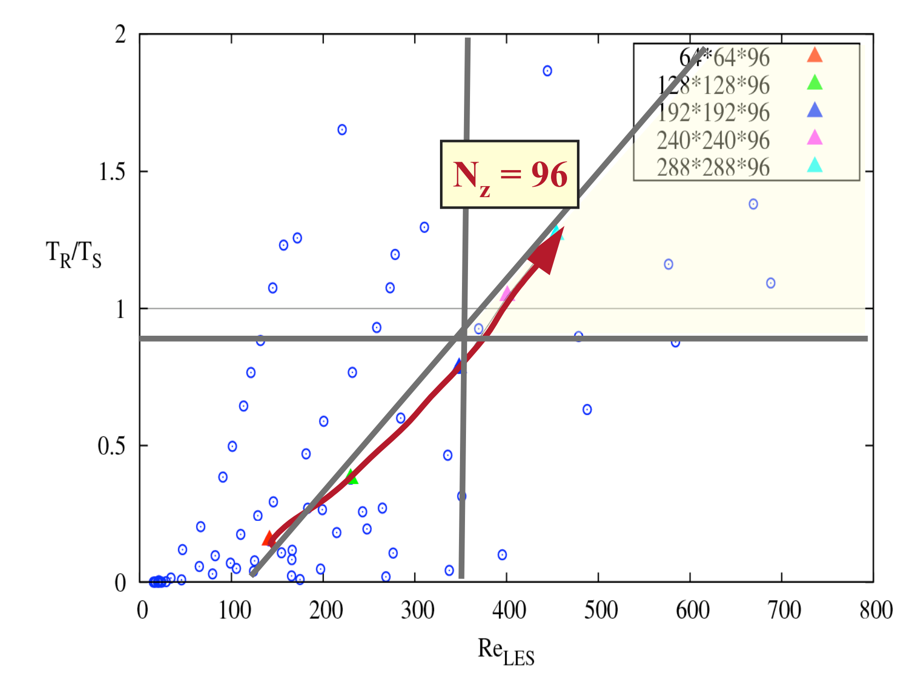
Designing High-Accuracy LES

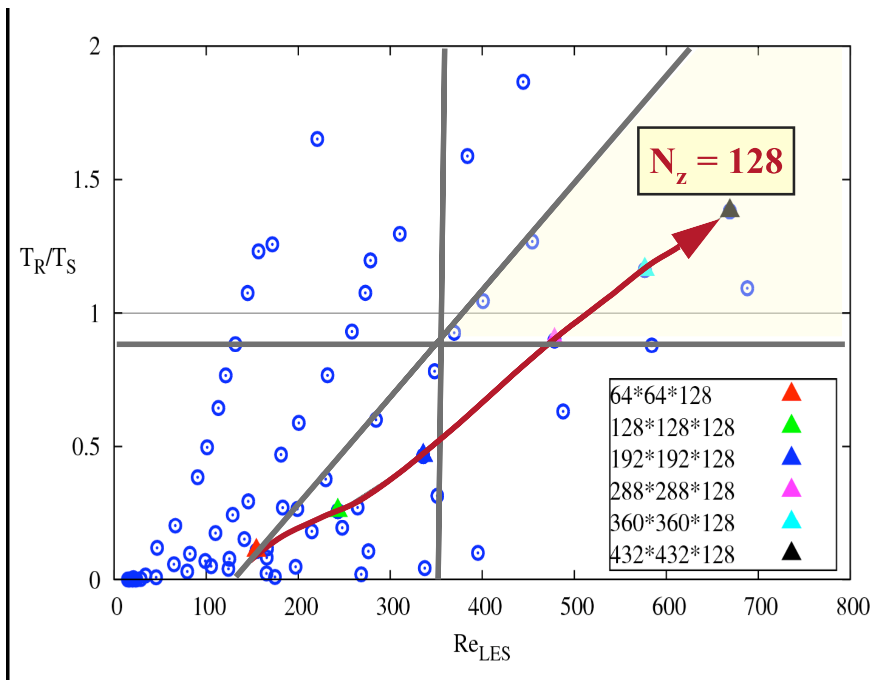
The $\Re - \mathrm{Re}_{LES}$ Parameter Space

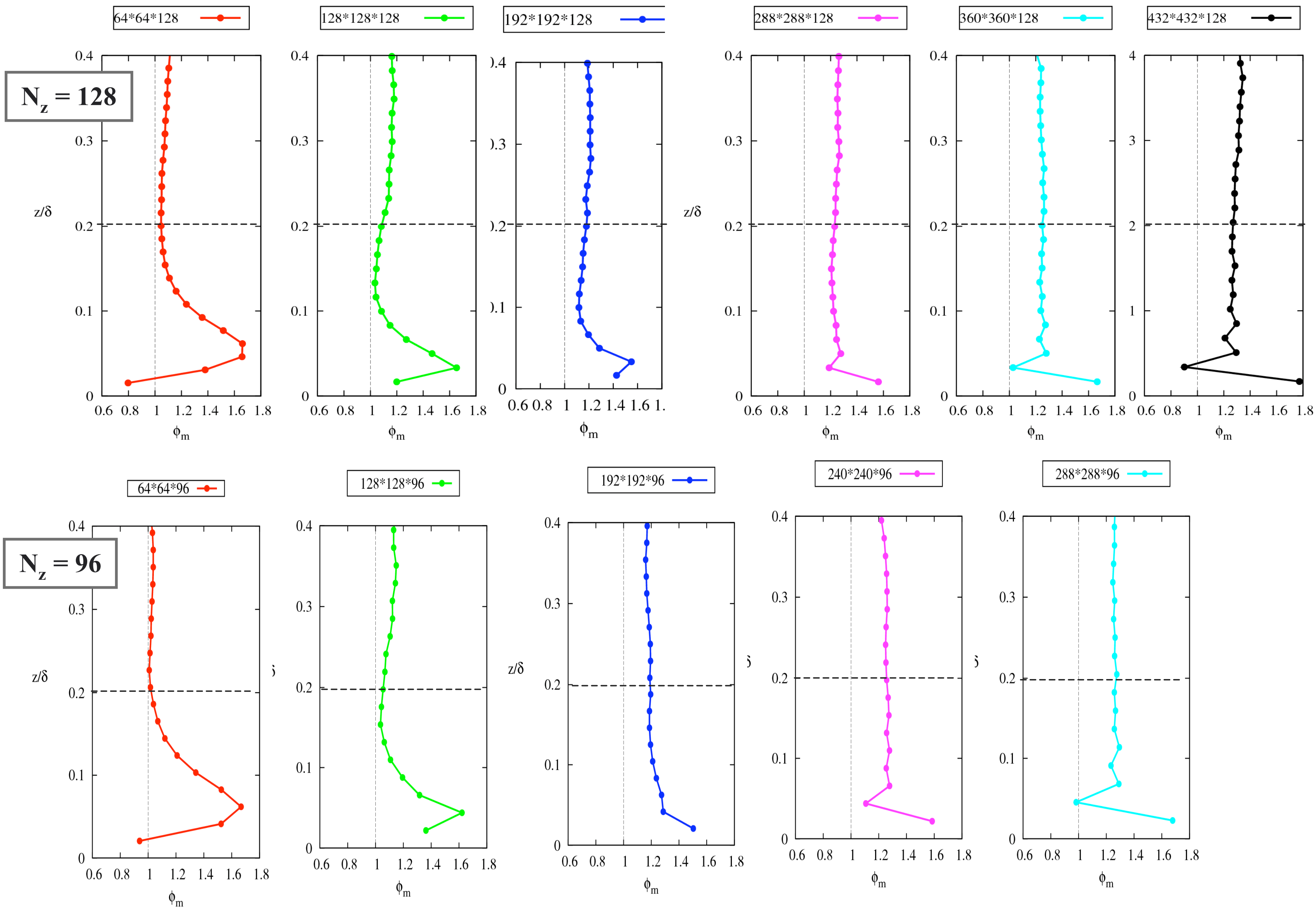
$$\Rightarrow \quad \frac{T_R}{T_S} \equiv \Re = \left(\frac{\xi \tilde{\kappa}_1}{N_\delta}\right) \mathrm{Re}_{LES} - 1$$

$$\mathrm{Re}_{LES} = \sqrt{2}\tilde{\kappa}_1 \frac{N_\delta}{C_S^2 (AR)^{4/3}}$$

$$\Re = \frac{\sqrt{2}\xi\tilde{\kappa}_1^2}{C_S^2 (AR)^{4/3}} - 1$$

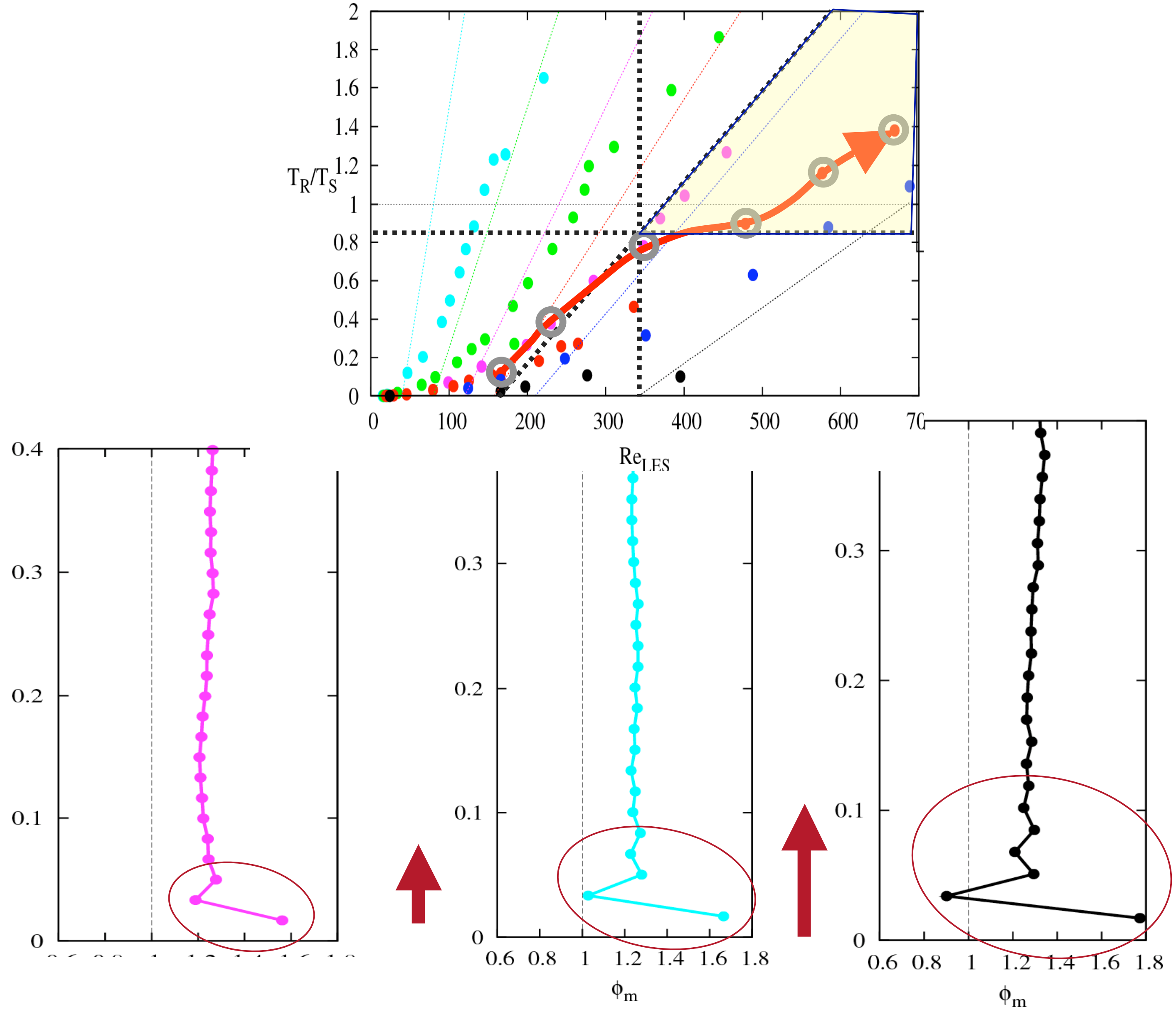






N_z = 128
N_z = 96
64*64*128
128*128*128
192*192*128
288*288*128
360*360*128
432*432*128
64*64*96
128*128*96
192*192*96
240*240*96
288*288*96
z/δ
φ_m

A Current Issue: Numerical Instability



Conclusions

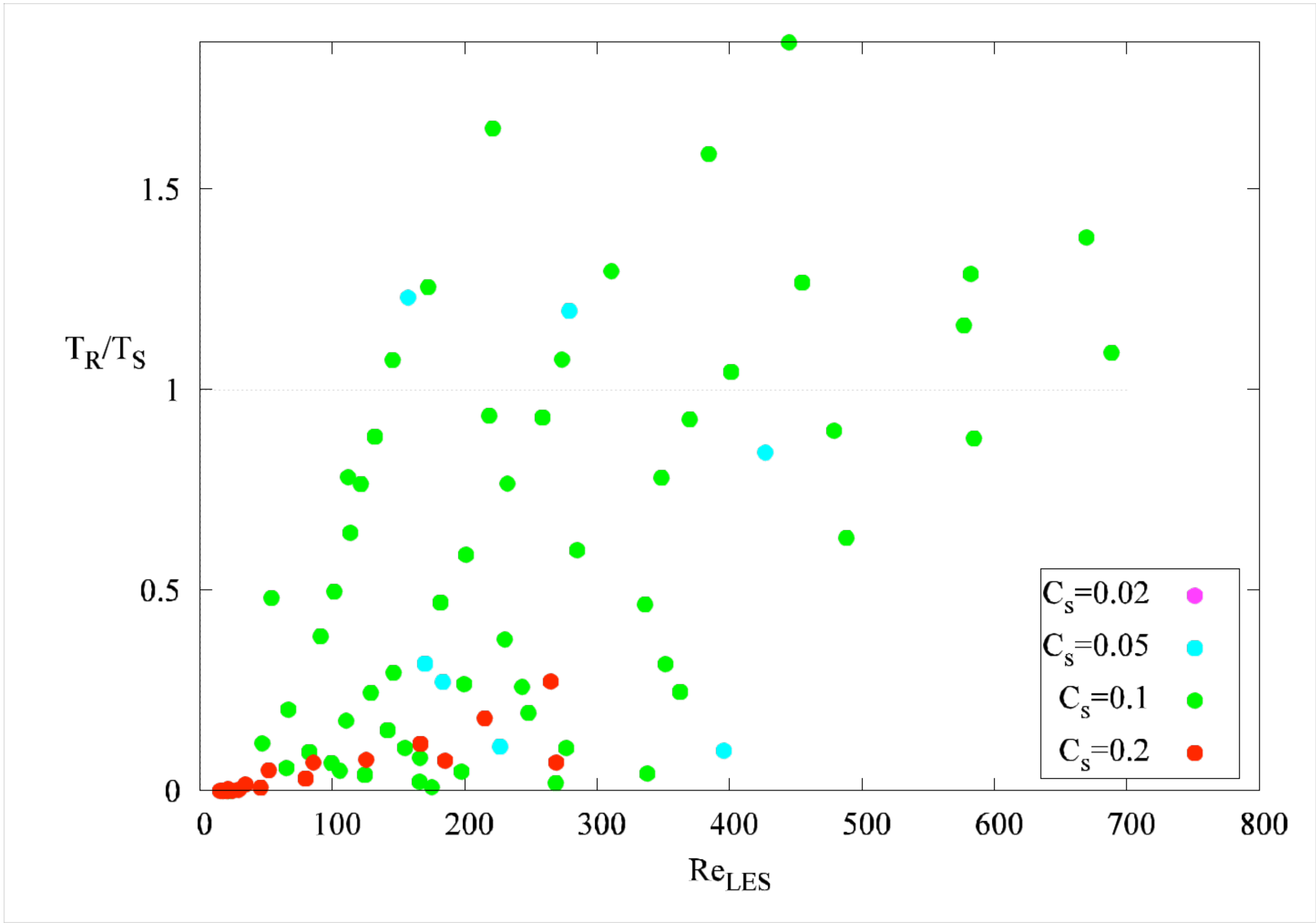
- **High-accuracy LES** ⇒
  1. removal of the overshoot in mean gradient
  2. sufficient resolution of the surface layer

- **We have created a framework** for developing high-accuracy LES: the $\mathfrak{R} - \mathrm{Re}_{LES}$ parameter space

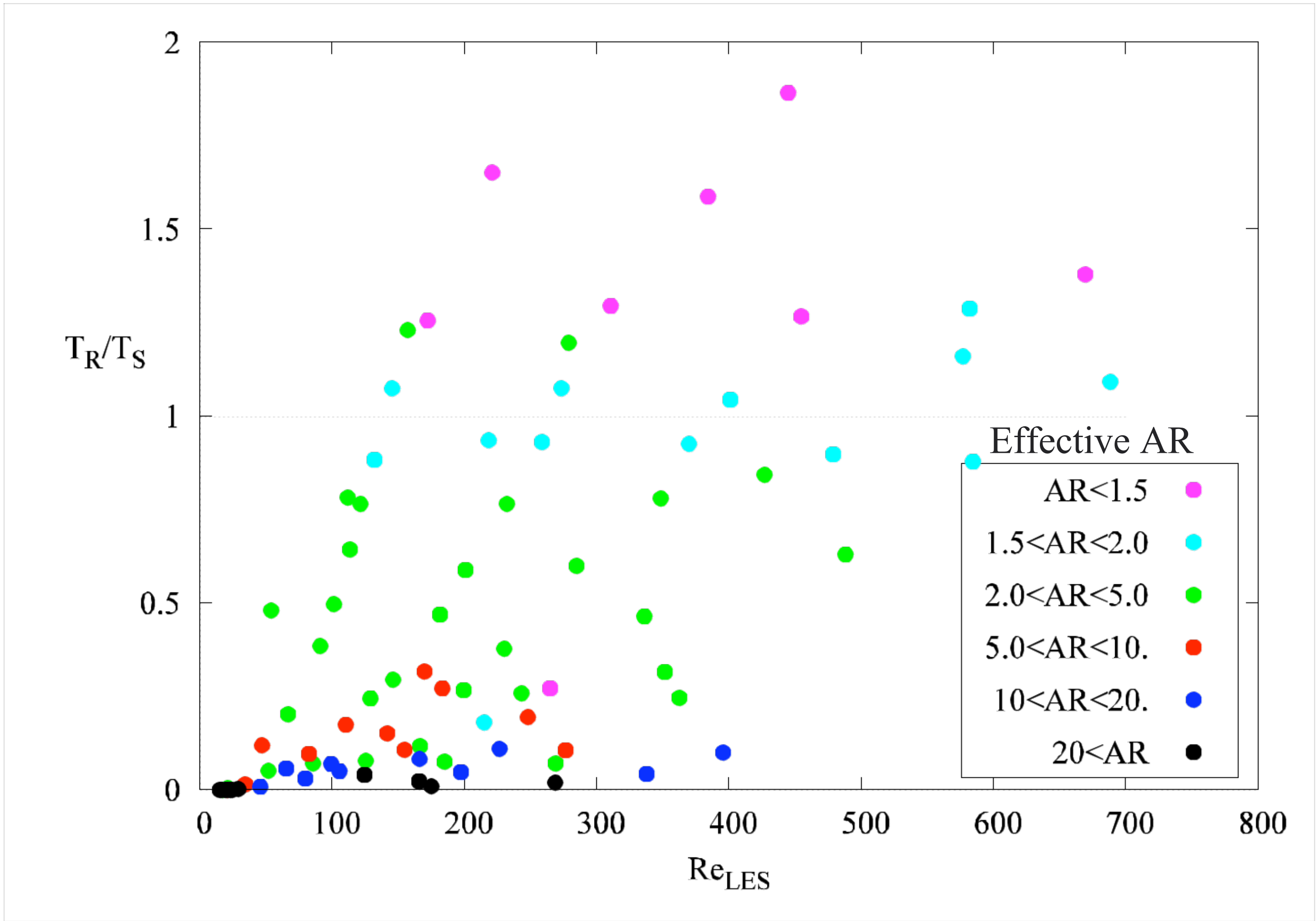
- **To create high-accuracy LES** the simulation must move into a "High-Accuracy Zone" (HAZ) through variation of
  - vertical grid resolution
  - grid aspect ratio
  - friction in model (e.g., model constant) and algorithm

- **Instability** arises as the simulation moves into the HAZ:
  - Tie will discuss next

Extra: Cs used in simulations



Extra: AR used in simulations



Note: For this plot, Tie used the effective AR based on explicit dealiasing filter. To get true AR, each of these should be divided by 1.5