Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

A rational length scale for large-eddy simulations on anisotropic grids

F.Xavier Trias[1], Jesús Ruano[1], Enrico Di Lavore[1]
Alexey Duben[2], Andrey Gorobets[2]

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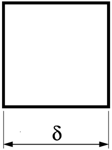

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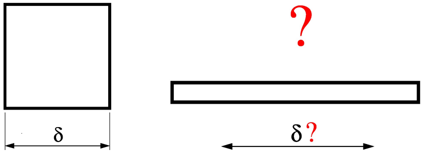

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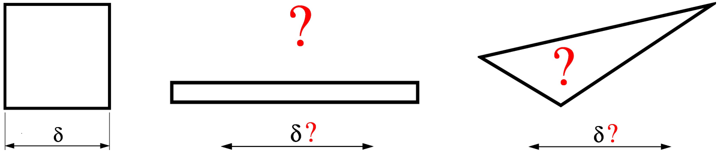
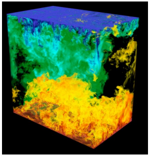


Contents

General motivation: (very) large-scale DNS/LES



DNS

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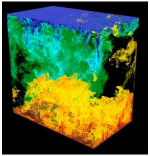


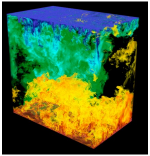
MareNostrum 5-ACC (Barcelona) | Snellius (Amsterdam) | TSUBAME4.0 (Tokyo)

MareNostrum 5-ACC (Barcelona)	Snellius (Amsterdam)	TSUBAME4.0 (Tokyo)
rank #8	rank #165	rank #31
1120 nodes with:	714 nodes with:	240 nodes with:
2× Intel Shappire Rapids 8460	2× AMD EPYC 9654 96C	2× AMD EPYC 9654 96-Core
1× NVIDIA Hopper 64 GB HBM	1× Infiniband NDR200	4× NVIDIA H100 SXM5
1× Infiniband NDR200		1× Infiniband NDR200

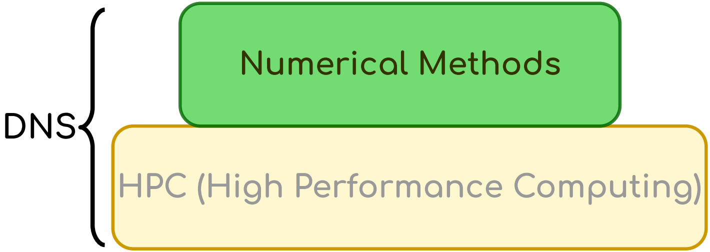
DNS

$\underbrace{}_{}$ **HPC (High Performance Computing)**

General motivation: (very) large-scale DNS/LES

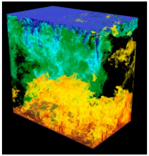


How to properly discretize NS?



General motivation: (very) large-scale DNS/LES

How to properly model SGS?



SGS models

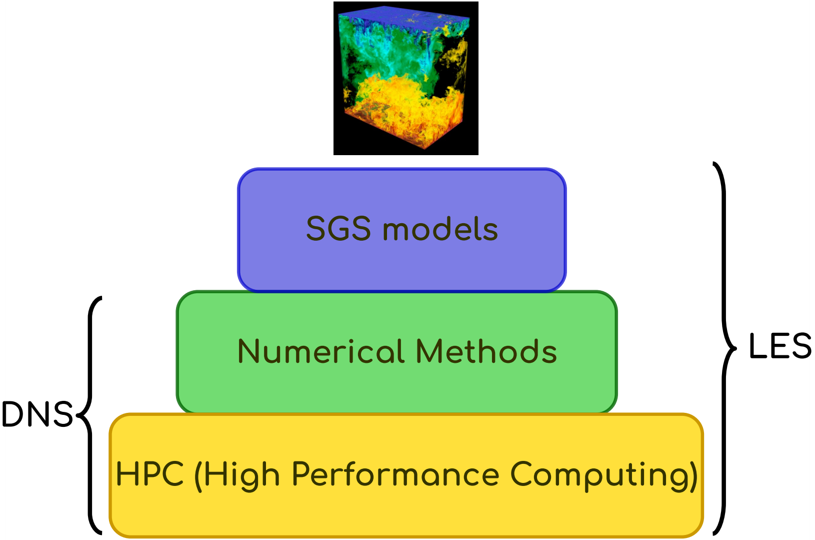
Numerical Methods

HPC (High Performance Computing)

DNS

LES

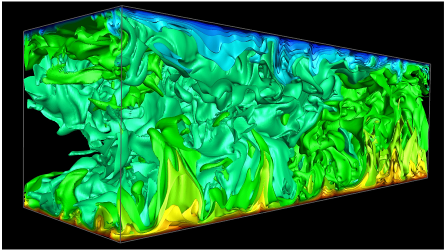
General motivation: (very) large-scale DNS/LES

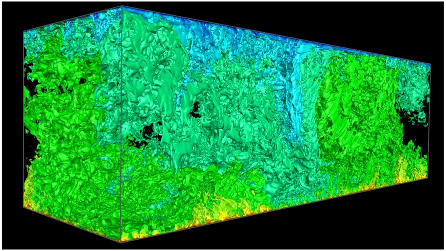


Motivation

Research question #1:

- What are we indeed solving with **finite volume method**?





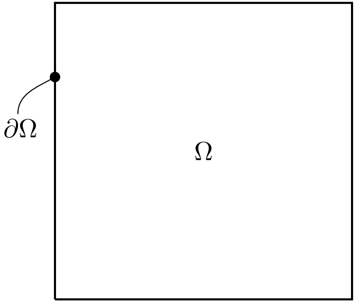
DNS[1] of air-filled Rayleigh–Bénard convection at $Ra = 10^8$ and 10^{10}

[1] B.Sanderse, F.X.Trias. *Energy-consistent discretization of viscous dissipation with application to natural convection flow*. **Computers & Fluids**, 286:106473, 2025

Motivation

Research question #2:

- What are we interpolating? What is the correct interpretation?



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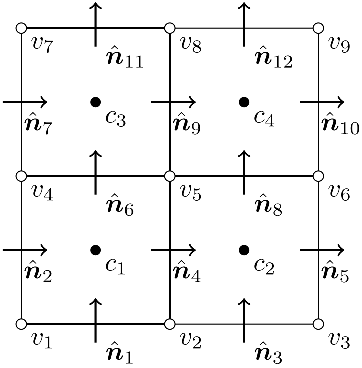

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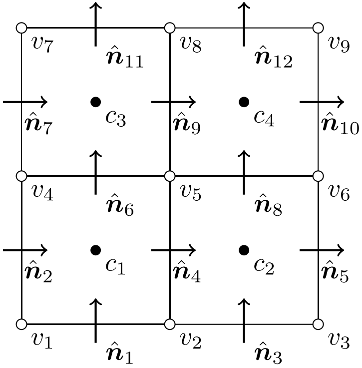
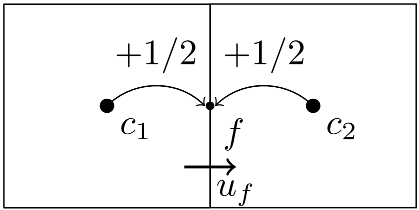
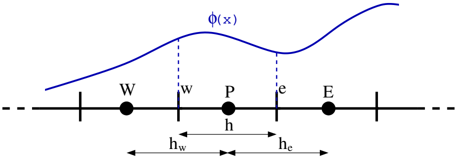




Revisiting FVM



Box filter: $$\overline{\phi}(x) = \frac{1}{h}\int_{x-h/2}^{x+h/2} \phi dx$$

$$\partial_x \overline{\phi}|_e = \overline{\partial_x \phi}|_e = (\phi_E - \phi_P)/h_e$$

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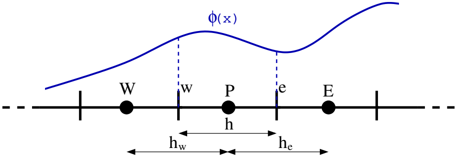

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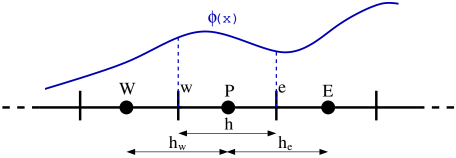

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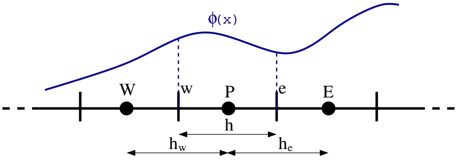

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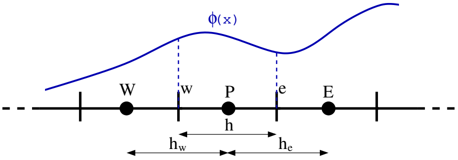

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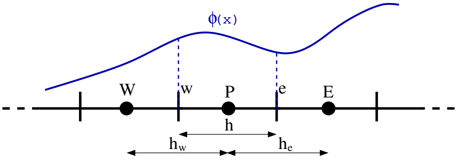

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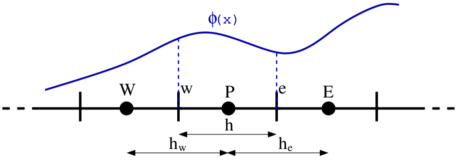

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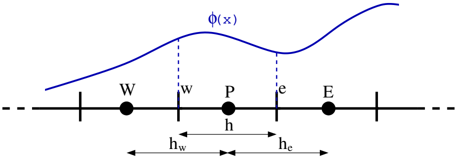

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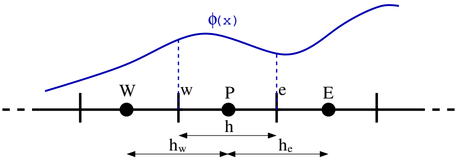
where $\tilde{\phi}_e = \frac{\overline{\phi}_P + \overline{\phi}_E}{2} = \overline{\phi}_e + \mathcal{O}(h^2)$

Revisiting FVM



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In summary (assuming that $\boldsymbol{u}$ is known):

$$\frac{\partial \overline{\phi}}{\partial t} + \overline{\frac{\partial (\boldsymbol{u}\phi)}{\partial x}} = \nu \overline{\frac{\partial^2 \phi}{\partial x^2}}$$

Instead, we are solving (in a 2^{nd}-order symmetry-preserving discretization):

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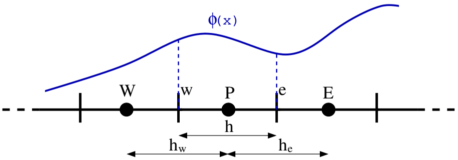
Revisiting FVM



Box filter: $\varphi \equiv \overline{\phi}(x) = \dfrac{1}{h}\displaystyle\int_{x-h/2}^{x+h/2} \phi dx$

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Subgrid characteristic length for LES: state of the art

$$\partial_t \overline{\boldsymbol{u}} + (\overline{\boldsymbol{u}} \cdot \nabla)\overline{\boldsymbol{u}} = \nabla^2 \overline{\boldsymbol{u}} - \nabla \overline{p} - \nabla \cdot \tau(\overline{\boldsymbol{u}}) \quad ; \qquad \nabla \cdot \overline{\boldsymbol{u}} = 0$$

$$\text{eddy-viscosity} \quad \longrightarrow \quad \tau \ (\overline{\boldsymbol{u}}) = -2\nu_t S(\overline{\boldsymbol{u}})$$

[2] F.X.Trias, D.Folch, A.Gorobets, A.Oliva. **Physics of Fluids**, 27: 065103, 2015.
[3] M.H.Silvis, R.A.Remmerswaal, R.Verstappen, **Physics of Fluids**, 29: 015105, 2017.

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$$\delta ?$$

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Subgrid characteristic length for LES: state of the art

- In the context of **LES**, most popular (by far) is:

$$\boxed{\delta_{\mathrm{vol}} = (\Delta x \Delta y \Delta z)^{1/3}} \Longleftarrow \textbf{Deardorff (1970)}$$

$$\delta_{\mathrm{Sco}} = f(a_1, a_2)\delta_{\mathrm{vol}}, \qquad \delta_{L^2} = \sqrt{(\Delta x^2 + \Delta y^2 + \Delta z^2)/3}$$

Subgrid characteristic length for LES: state of the art

- In the context of **LES**, most popular (by far) is:

$$\boxed{\delta_{\mathrm{vol}} = (\Delta x \Delta y \Delta z)^{1/3}} \Longleftarrow \textbf{Deardorff (1970)}$$

$$\delta_{\mathrm{Sco}} = f(a_1, a_2)\delta_{\mathrm{vol}}, \qquad \delta_{L^2} = \sqrt{(\Delta x^2 + \Delta y^2 + \Delta z^2)/3}$$

$$\delta_{\mathrm{lsq}} = \sqrt{\frac{\hat{\mathsf{G}}\hat{\mathsf{G}}^T : \mathsf{G}\mathsf{G}^T}{\mathsf{G}\mathsf{G}^T : \mathsf{G}\mathsf{G}^T}} \Longleftarrow \textbf{Trias et al. (2017)}$$

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- In the context of **DES**:

$$\boxed{\delta_{\mathrm{max}} = \max(\Delta x, \Delta y, \Delta z)} \Longleftarrow \textbf{Sparlart et al. (1997)}$$

Flow-dependant definitions

$$\delta_{\boldsymbol{\omega}} = \sqrt{(\omega_x^2 \Delta y \Delta z + \omega_y^2 \Delta x \Delta z + \omega_z^2 \Delta x \Delta y)/|\boldsymbol{\omega}|^2} \Longleftarrow \textbf{Chauvet et al. (2007)}$$

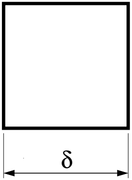
$$\tilde{\delta}_{\boldsymbol{\omega}} = \frac{1}{\sqrt{3}} \max_{n,m=1,\dots,8} |\boldsymbol{l}_n - \boldsymbol{l}_m| \Longleftarrow \textbf{Mockett et al. (2015)}$$

$$\delta_{\mathrm{SLA}} = \tilde{\delta}_{\boldsymbol{\omega}} F_{\mathrm{KH}}(VTM) \Longleftarrow \textbf{Shur et al. (2015)}$$

A rational length scale for LES

Research question #3:

- Can we establish a **simple**, **robust**, and **easily implementable** definition of δ for any type of grid that minimizes the impact of mesh anisotropies on the performance of subgrid-scale models?



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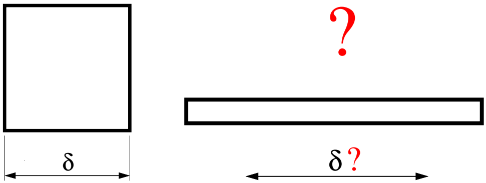

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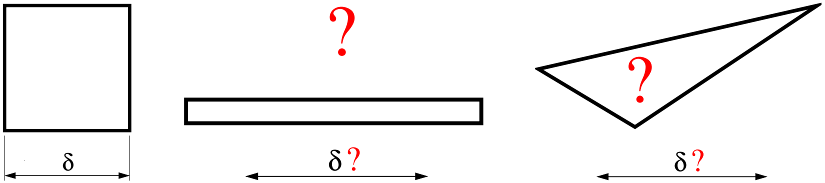

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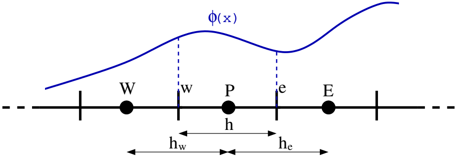
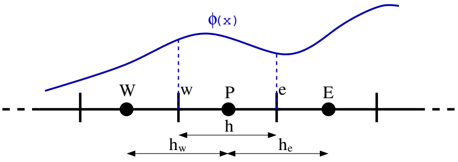


Box filter: $$\overline{\phi}(x) = \frac{1}{h}\int_{x-h/2}^{x+h/2} \phi dx$$

$$\partial_x\overline{\phi} = \overline{\partial_x\phi} = (\phi_e - \phi_w)/h$$

Remark #1: the actual filter length, δ, when computing the face derivative is h_e, *i.e.*, the distance between the adjacent nodes P and E.

A rational length scale for LES



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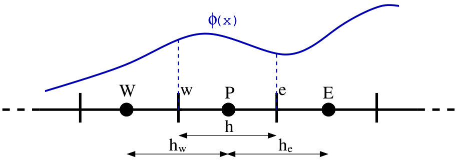
The diffusive term in a FVM framework is approximated as follows

$$\left.\frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right)\right|_P \approx \frac{1}{h}\left(\Gamma \left.\frac{\partial \phi}{\partial x}\right|_e - \Gamma \left.\frac{\partial \phi}{\partial x}\right|_w\right) = \left.\overline{\frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right)}\right|_P$$

A rational length scale for LES



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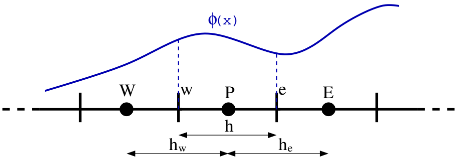

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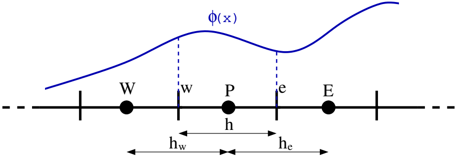

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Remark #1: the actual filter length, δ, when computing the face derivative is h_e, *i.e.*, the distance between the adjacent nodes P and E.

Remark #2: two filtering operations are performed when computing the diffusive term:

- the calculation of the face derivative
- the cell-to-face interpolation of Γ

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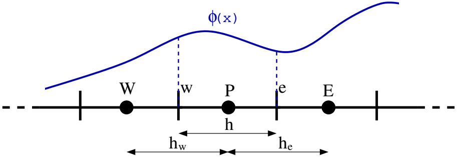
A rational length scale for LES



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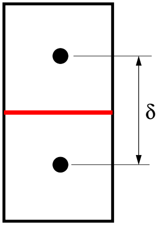
Both filtering operators share the same filter length, δ; namely, the distance between the nodes adjacent to the corresponding **face**.



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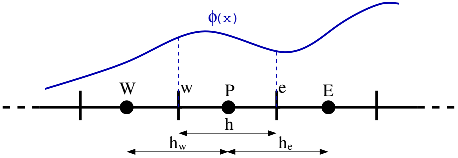

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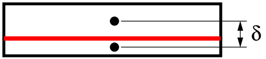

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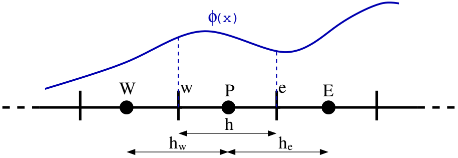

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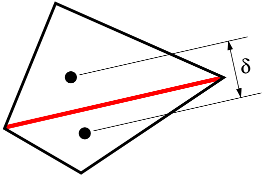

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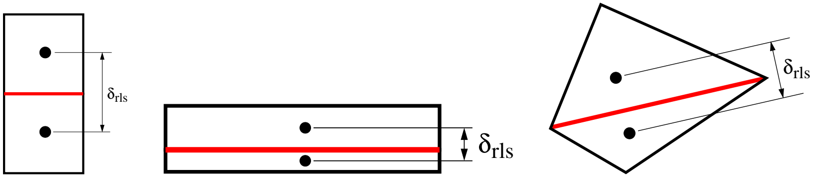
A rational length scale

Properties of new definition, δ_{rls}



A rational length scale

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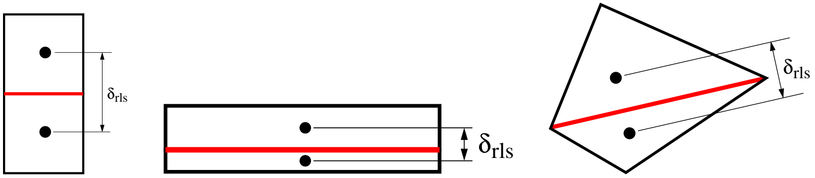

- Locally defined

A rational length scale

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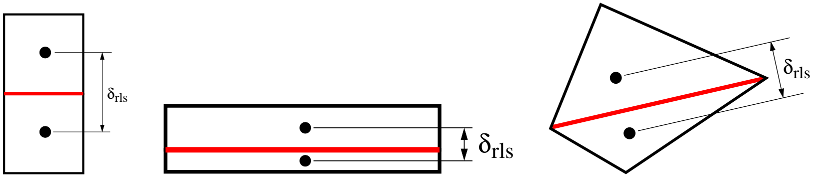
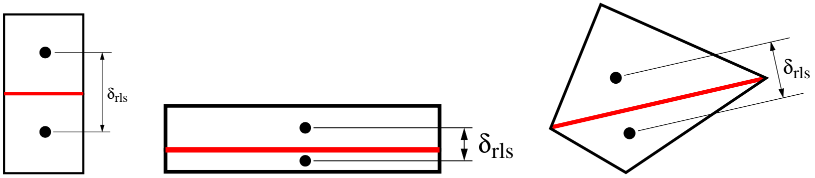


- Locally defined
- Well-bounded: $\Delta x \leqslant \delta_{\mathrm{rls}} \leqslant \Delta z$ (assuming $\Delta x \leqslant \Delta y \leqslant \Delta z$)

A rational length scale

Properties of new definition, δ_{rls}



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- Sensitive to flow orientation, *e.g.* shear layers

A rational length scale

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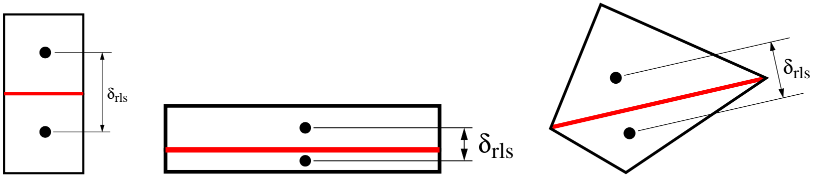

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- Applicable to unstructured grids

A rational length scale

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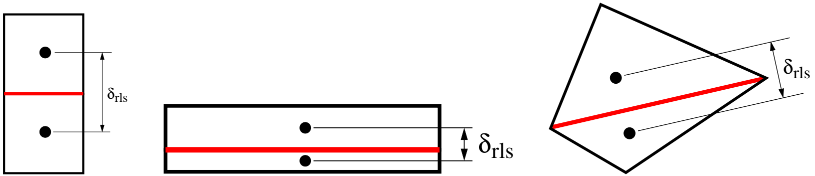

- Locally defined
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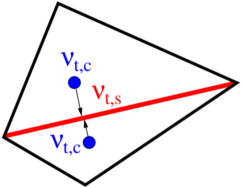
- Sensitive to flow orientation, *e.g.* shear layers
- Applicable to unstructured grids
- Easy and cheap

A rational length scale

Implementation and an alternative definition

$$\nu_{t,c} \xrightarrow{\text{interpolation}} \nu_{t,s}$$



$$\nu_{t,c} \dashrightarrow \hat{\nu}_{t,c} \longrightarrow \hat{\nu}_{t,s} \dashrightarrow \nu_{t,s}$$

A rational length scale

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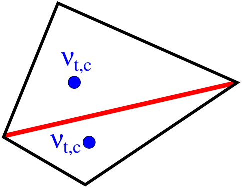

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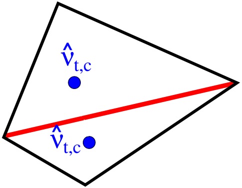
Implementation and an alternative definition

$$\nu_{t,c} \xrightarrow{\text{interpolation}} \nu_{t,s}$$

$$\nu_{t,c} \overset{1/\delta_{vol}^2}{\dashrightarrow} \hat{\nu}_{t,c} \longrightarrow \hat{\nu}_{t,s} \dashrightarrow \nu_{t,s}$$



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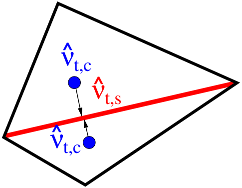
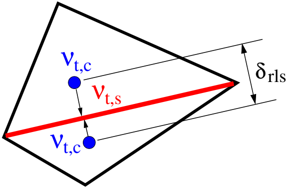


$$\nu_{t,c} \xrightarrow{1/\delta^2_{vol}} \hat{\nu}_{t,c} \xrightarrow{\text{interpolation}} \hat{\nu}_{t,s} \dashrightarrow \nu_{t,s}$$

A rational length scale

Implementation and an alternative definition

$$\nu_{t,c} \xrightarrow{\text{interpolation}} \nu_{t,s}$$



$$\nu_{t,c} \xrightarrow{1/\delta_{vol}^2} \hat{\nu}_{t,c} \xrightarrow{\text{interpolation}} \hat{\nu}_{t,s} \xrightarrow{\delta_{rls}^2} \nu_{t,s}$$

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Implementation and an alternative definition

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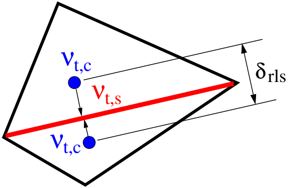

We can also compute an equivalent filter length, $\tilde{\delta}_{\mathrm{rls}}$, that leads to the same local dissipation

$$\tilde{\delta}_{\mathrm{rls}}^2 \hat{\nu}_t \mathsf{G} : \mathsf{G} = \hat{\nu}_t \hat{\mathsf{G}} : \hat{\mathsf{G}}$$

where $\hat{\mathsf{G}} \equiv \mathsf{G}\Delta$ and $\Delta \equiv \mathrm{diag}(\Delta x, \Delta y, \Delta x)$.

A rational length scale

Implementation and an alternative definition

$$\nu_{t,c} \xrightarrow{\text{interpolation}} \nu_{t,s}$$

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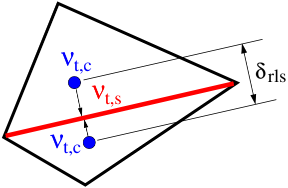

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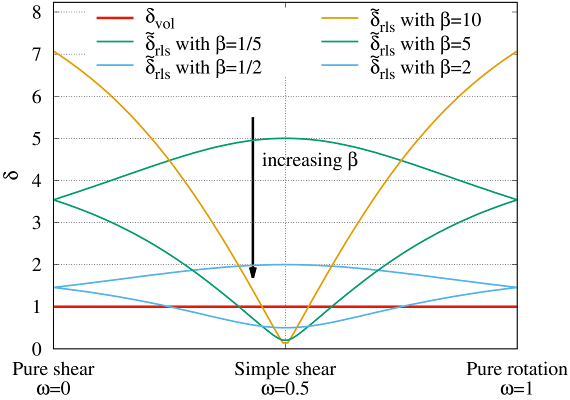
$$\tilde{\delta}^2_{\mathrm{rls}} \hat{\nu}_t \mathsf{G} : \mathsf{G} = \hat{\nu}_t \hat{\mathsf{G}} : \hat{\mathsf{G}} \quad \Longrightarrow \quad \boxed{\tilde{\delta}_{\mathrm{rls}} = \sqrt{\frac{\hat{\mathsf{G}} : \hat{\mathsf{G}}}{\mathsf{G} : \mathsf{G}}} = \sqrt{\frac{\mathrm{tr}(\hat{\mathsf{G}}\hat{\mathsf{G}}^T)}{\mathrm{tr}(\mathsf{G}\mathsf{G}^T)}}}$$

where $\hat{\mathsf{G}} \equiv \mathsf{G}\Delta$ and $\Delta \equiv \mathrm{diag}(\Delta x, \Delta y, \Delta x)$.

A rational length scale

Properties of new definition $\tilde{\delta}_{\mathrm{rls}}$

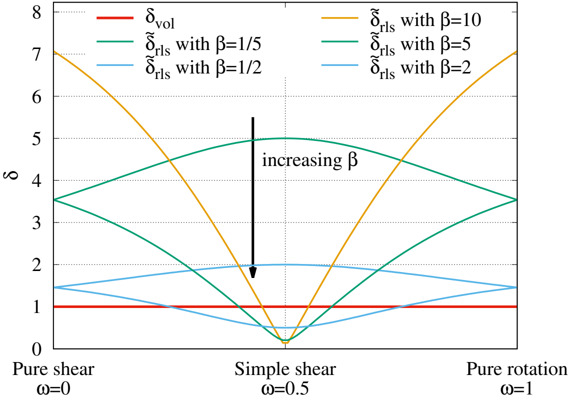
$$\Delta = \begin{pmatrix} \Delta x & 0 \\ 0 & \Delta y \end{pmatrix} \qquad G = \begin{pmatrix} \partial_x u & \partial_y u \\ \partial_y u & \partial_y v \end{pmatrix}$$



A rational length scale

Properties of new definition $\tilde{\delta}_{\mathrm{rls}}$

$$\Delta = \begin{pmatrix} \Delta x & 0 \\ 0 & \Delta y \end{pmatrix} = \begin{pmatrix} \beta & 0 \\ 0 & \beta^{-1} \end{pmatrix} \quad G = \begin{pmatrix} \partial_x u & \partial_y u \\ \partial_y u & \partial_y v \end{pmatrix}$$



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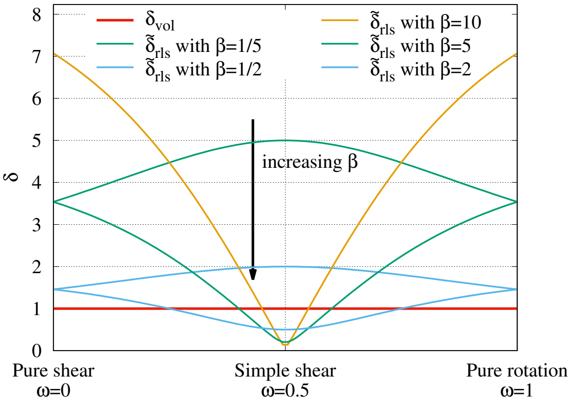

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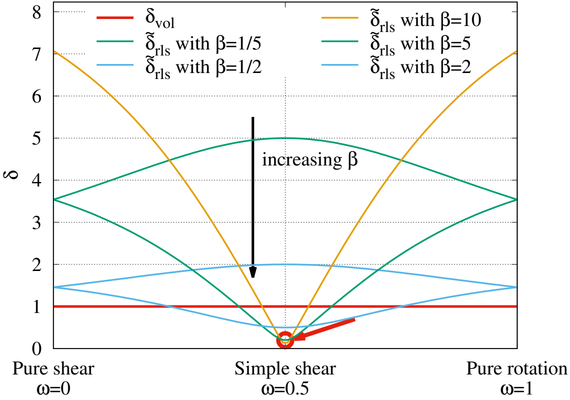
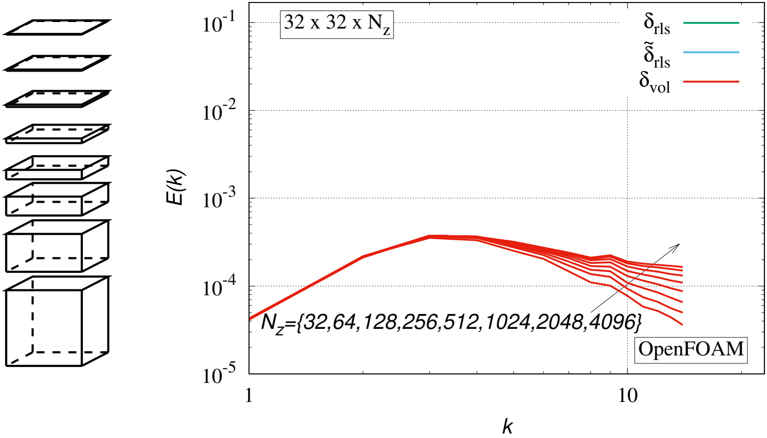


A rational length scale

Isotropic turbulence on anisotropic grids

Comparison with classical Comte-Bellot & Corrsin (CBC) experiment



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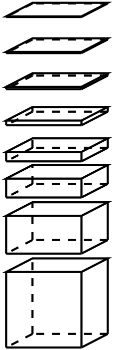

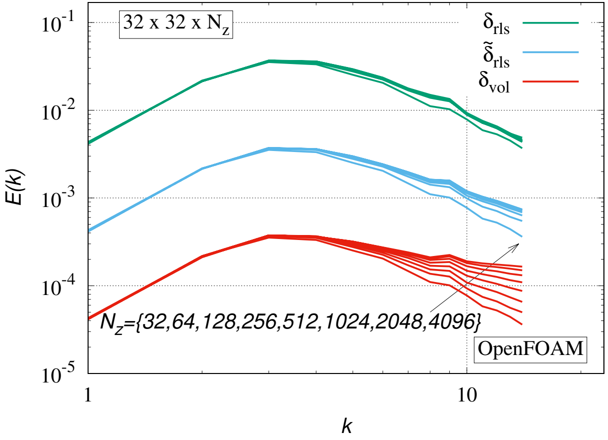

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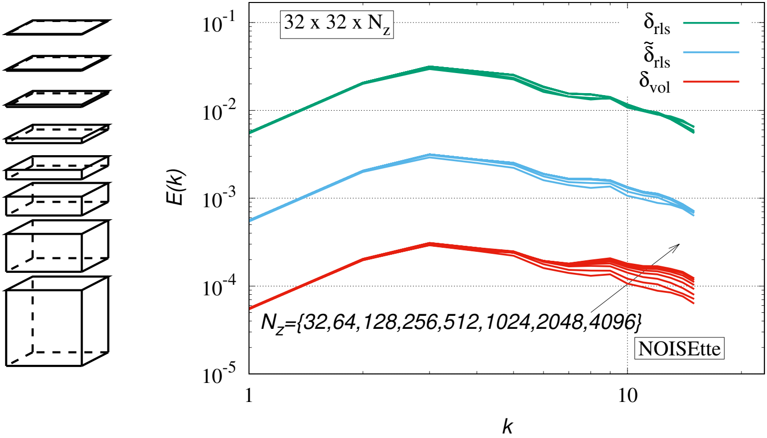

A rational length scale

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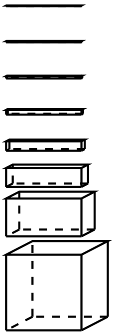
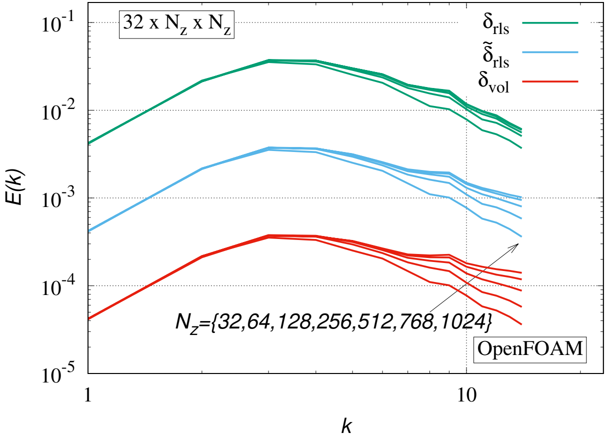
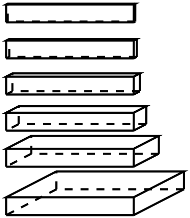


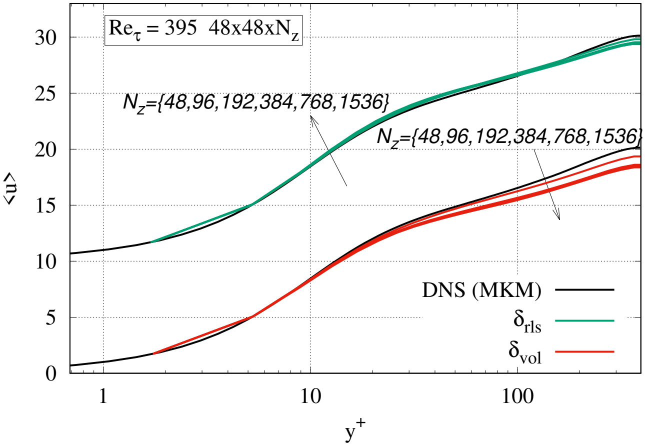


A rational length scale

Turbulent channel flow at $Re_\tau = 395$

Average velocity $48 \times 48 \times N_z$

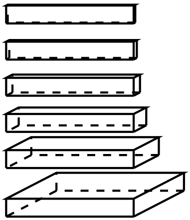


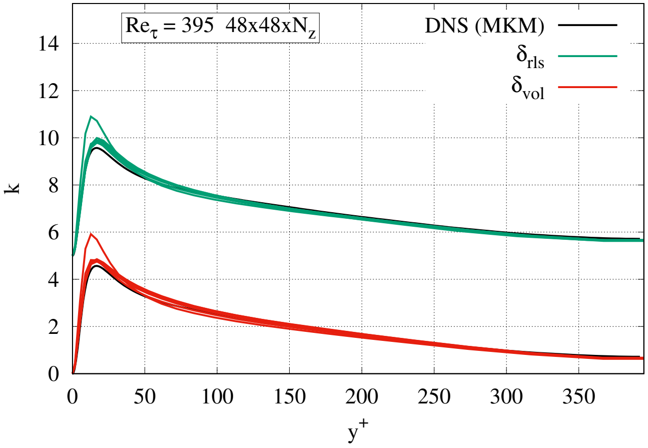


A rational length scale

Turbulent channel flow at $Re_\tau = 395$

Turbulent kinetic energy $\quad 48 \times 48 \times N_z$

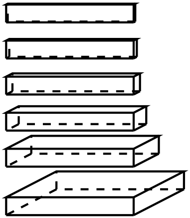


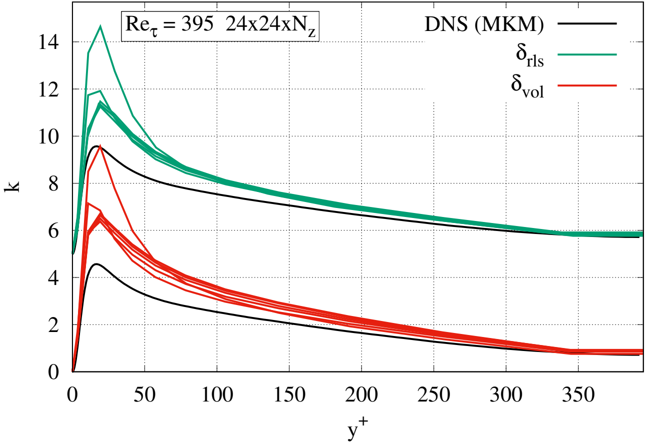


A rational length scale

Turbulent channel flow at $Re_\tau = 395$

Turbulent kinetic energy $\quad 24 \times 24 \times N_z$

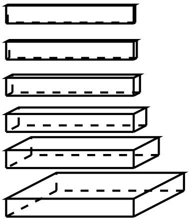


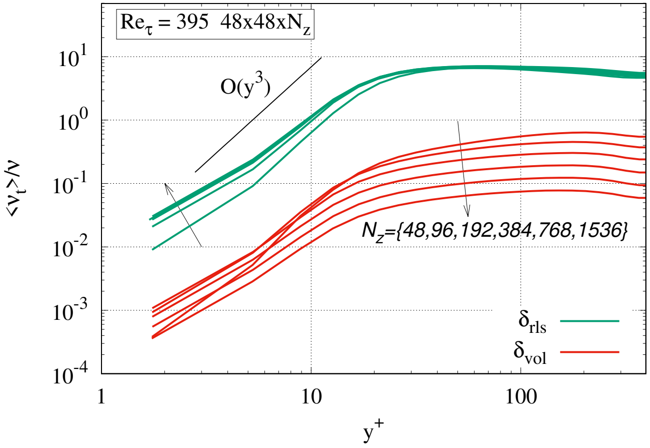


A rational length scale

Turbulent channel flow at $Re_\tau = 395$

Turbulent viscosity $48 \times 48 \times N_z$





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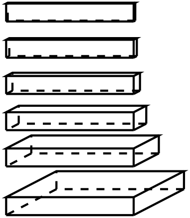
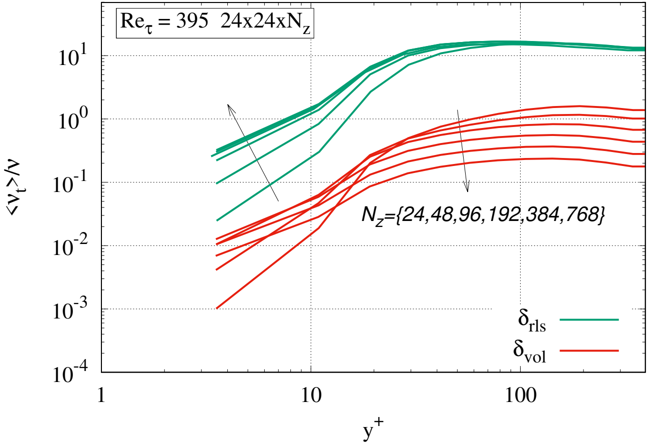
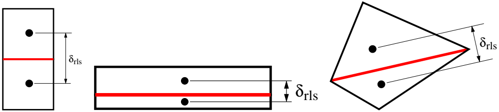




Concluding remarks

- A new definition for δ has been proposed



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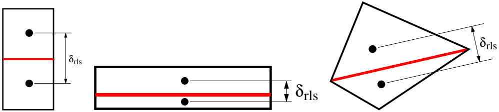

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- Suitable for unstructured grids

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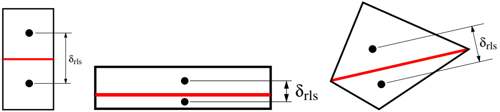

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  - HIT ✓
  - Turbulent channel flow ✓
  - Unstructured grids (on-going)

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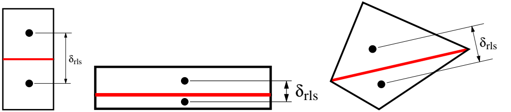

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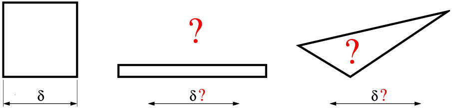
Takeaway message:



- Definition of δ can have a big effect on simulation results

Thank you for your attendance

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A rational length scale for large-eddy simulation of turbulence on anisotropic grids

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ABSTRACT

Due to the prohibitive cost of resolving all relevant scales, direct numerical simulations of turbulence remain unfeasible for most real-world applications. Consequently, dynamically simplified formulations are needed for coarse-grained simulations. In this regard, eddy-viscosity models for large-eddy simulation (LES) are widely used in both academia and industry. These models require a subgrid characteristic length, typically linked to the local grid size. While this length scale corresponds to the mesh step for isotropic grids, its definition for unstructured

https://github.com/jruanoperez/DHIT