Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

A discretization-consistent length scale definition for large-eddy simulations of complex flows

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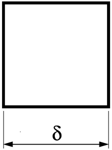

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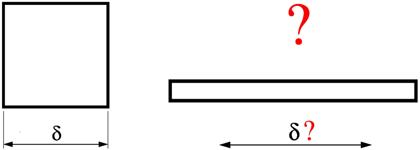

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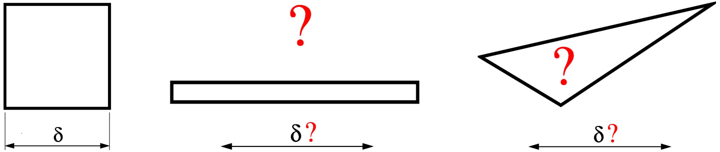
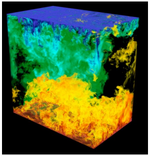


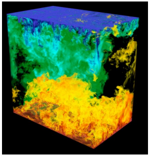
Contents

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

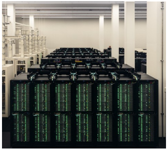


DNS{

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

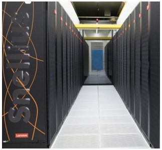


MareNostrum 5-ACC
(Barcelona)



rank #8
1120 nodes with:
2× Intel Shappire Rapids 8460
1× NVIDIA Hopper 64 GB HBM
1× Infiniband NDR200

Snellius
(Amsterdam)



rank #165
714 nodes with:
2× AMD EPYC 9654 96C
1× Infiniband NDR200

TSUBAME4.0
(Tokyo)

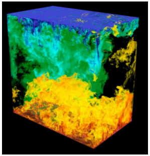
rank #31
240 nodes with:
2× AMD EPYC 9654 96-Core
4× NVIDIA H100 SXM5
1× Infiniband NDR200

intel XEON PLATINUM inside

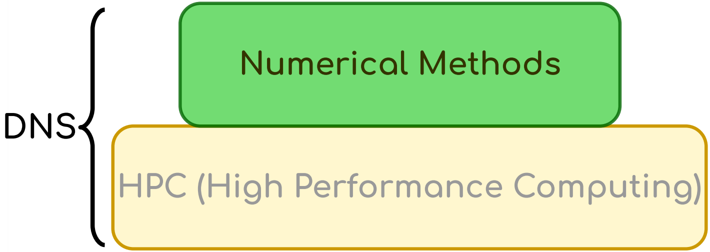
DNS

HPC (High Performance Computing)

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

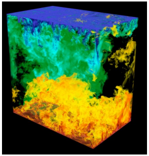


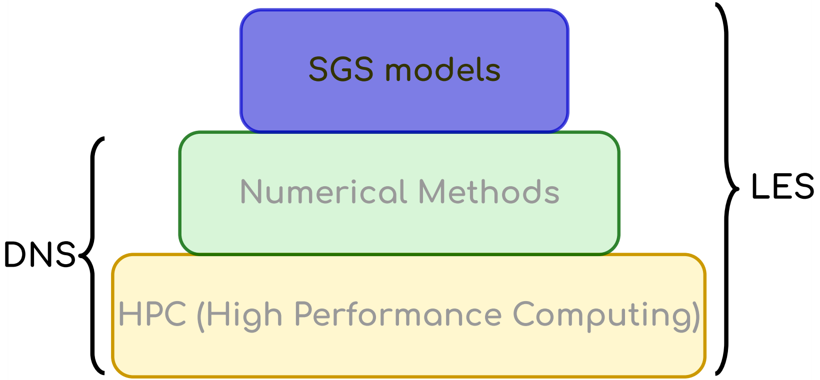
How to properly discretize NS?



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

How to properly model SGS?





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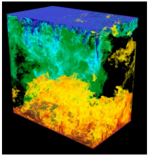
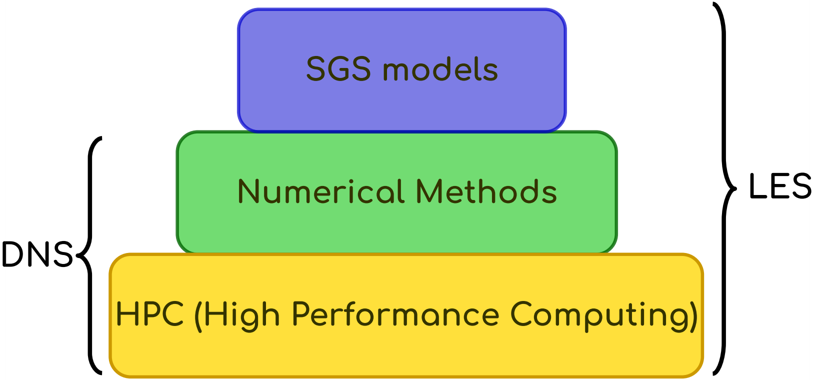
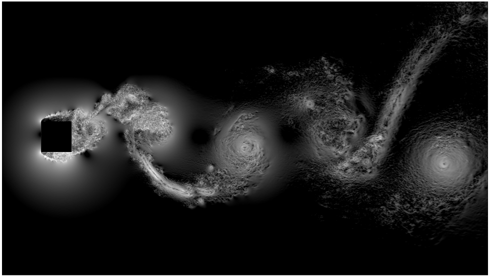


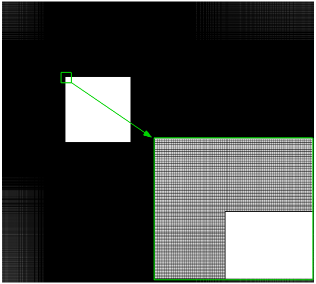


Motivation

Research question #1:

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





DNS[1] of the flow around a square cylinder at $Re = 55000$ (2.6B grid points)

[1] F.X.Trias, À.Alsalti, A.Oliva. *On the Reynolds-number scaling of Poisson solver complexity*, **Physics of Fluids**, 38 (4):045157, 2026. arXiv: 2512.22644

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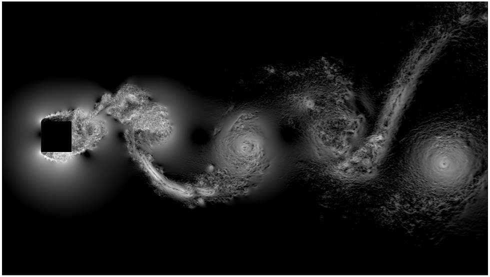

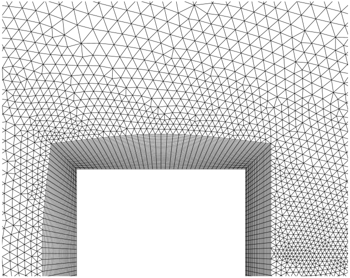

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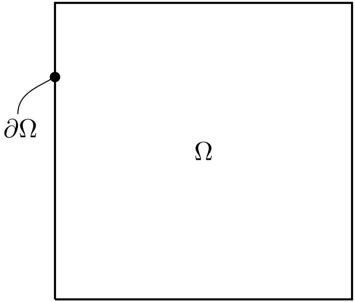

Motivation

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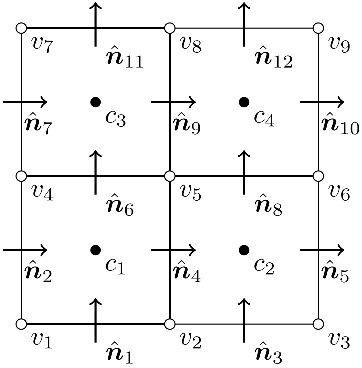

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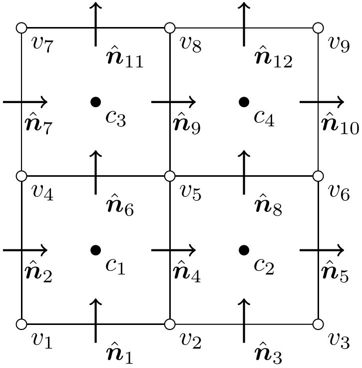
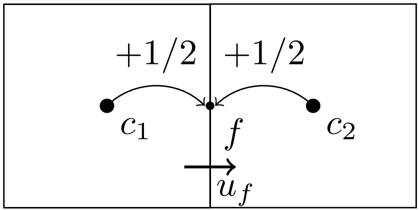
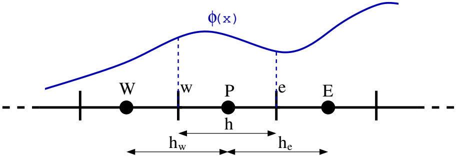




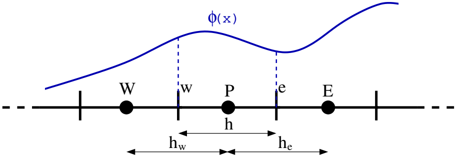
Revisiting FVM



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

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

Revisiting FVM



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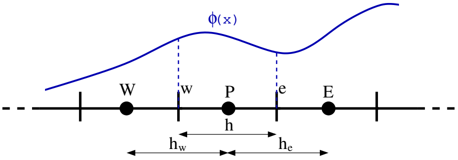
Revisiting FVM



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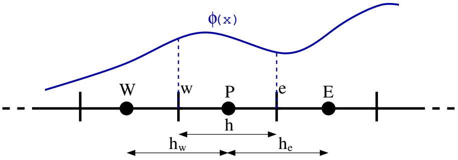
Exact FVM eq!

Revisiting FVM



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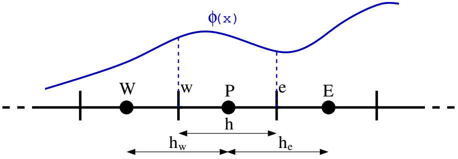
Exact FVM eq!

$$h\frac{\partial \overline{\phi}_P}{\partial t} + (\boldsymbol{u}\phi)_e - (\boldsymbol{u}\phi)_w = \nu \left(\left.\frac{\partial \phi}{\partial x}\right|_e - \left.\frac{\partial \phi}{\partial x}\right|_w \right)$$

Revisiting FVM



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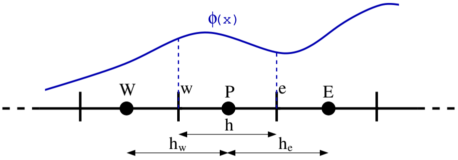

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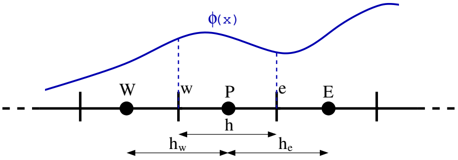

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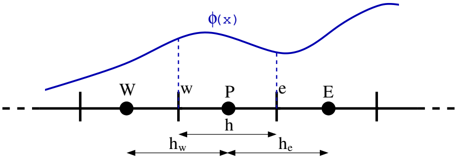
$$\boxed{\frac{\partial \overline{\phi}}{\partial t} + \overline{\frac{\partial (\boldsymbol{u}\tilde{\overline{\phi}})}{\partial x}} = \nu \overline{\frac{\partial^2 \overline{\overline{\phi}}}{\partial x^2}}}$$

Revisiting FVM



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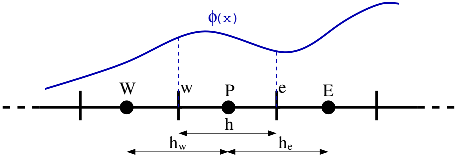
$$\boxed{\frac{\partial \overline{\phi}}{\partial t} + \overline{\frac{\partial (\boldsymbol{u}\widetilde{\overline{\phi}})}{\partial x}} = \nu \overline{\frac{\partial^2 \overline{\overline{\phi}}}{\partial x^2}}}$$

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

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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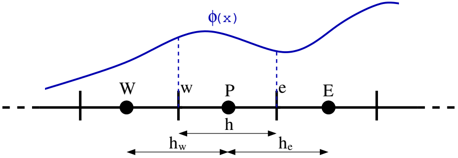
Revisiting FVM



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

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Exact FVM eq!

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Approx FVM eq!

Subgrid characteristic length for LES: state of the art

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

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

[3] F.X.Trias, D.Folch, A.Gorobets, A.Oliva. **Physics of Fluids**, 27: 065103, 2015.

[4] M.H.Silvis, R.A.Remmerswaal, R.Verstappen, **Physics of Fluids**, 29: 015105, 2017.

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$D_m(\overline{u}) \longrightarrow$ Smagorinsky (1963), WALE (1999), Vreman (2004), QR-model (2011), σ-model (2011), S3PQR[3] (2015), vortex-stretching-based model[4] (2017)

[3] F.X.Trias, D.Folch, A.Gorobets, A.Oliva. **Physics of Fluids**, 27: 065103, 2015.
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$D_m(\overline{u}) \longrightarrow$ Smagorinsky (1963), WALE (1999), Vreman (2004), QR-model (2011), σ-model (2011), S3PQR[3] (2015), vortex-stretching-based model[4] (2017)

$C_m \longrightarrow$ Germano's dynamic model (1991), Lagrangian dynamic (1995), Global dynamic approach (2006)

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[3] F.X.Trias, D.Folch, A.Gorobets, A.Oliva. **Physics of Fluids**, 27: 065103, 2015.

[4] M.H.Silvis, R.A.Remmerswaal, R.Verstappen, **Physics of Fluids**, 29: 015105, 2017.

Subgrid characteristic length for LES: state of the art

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

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Subgrid characteristic length for LES: state of the art

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

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

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

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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

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

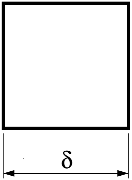
$$\tilde{\delta}_{\boldsymbol{\omega}} = \frac{1}{\sqrt{3}} \max_{n,m=1,\dots,8} |\boldsymbol{l}_n - \boldsymbol{l}_m| \Longleftarrow \textbf{Mockett et al. (2015)}$$

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

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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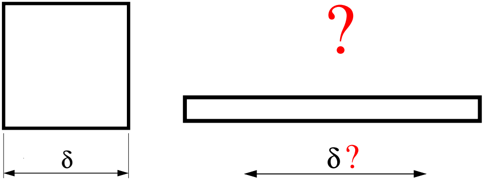

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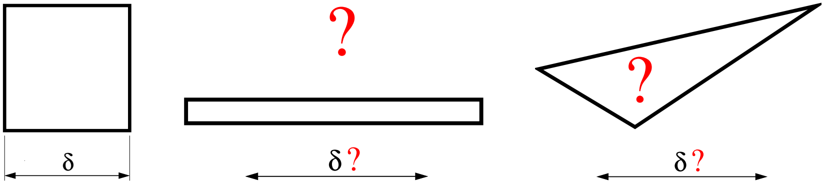

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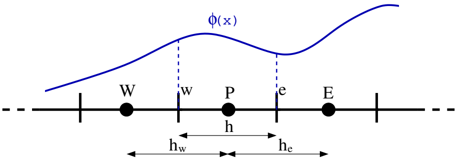

Box filter: $$\overline{\phi}(x) = \frac{1}{h}\int_{x-h/2}^{x+h/2} \phi dx$$

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

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.

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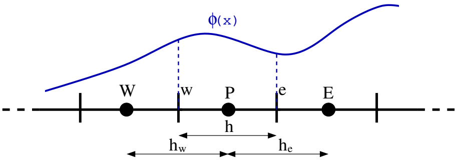

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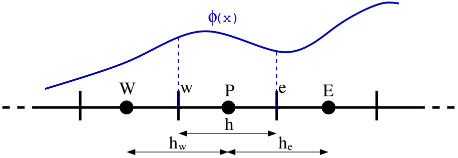
The diffusive term in a FVM framework is approximated as follows

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

A rational length scale for LES



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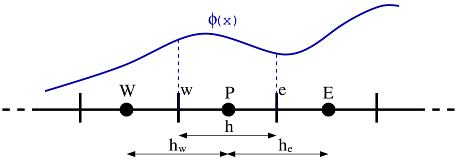

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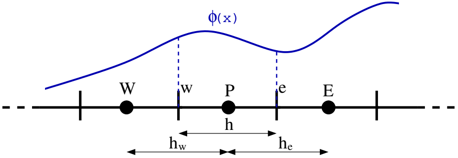
$$\approx \frac{1}{h}\left(\frac{\Gamma_E+\Gamma_P}{2}\frac{\phi_E-\phi_P}{h_e} - \frac{\Gamma_P+\Gamma_W}{2}\frac{\phi_P-\phi_W}{h_w}\right) = \overline{\frac{\partial}{\partial x}\left(\overline{\Gamma}\frac{\overline{\partial\phi}}{\partial x}\right)}\bigg|_P$$

A rational length scale for LES



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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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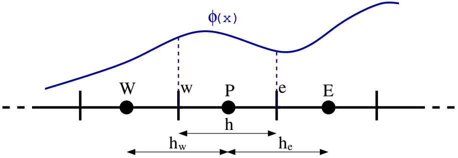
A rational length scale for LES



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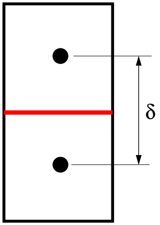
Both filtering operators share the same filter length, δ; namely, the distance between the nodes adjacent to the corresponding **face**.



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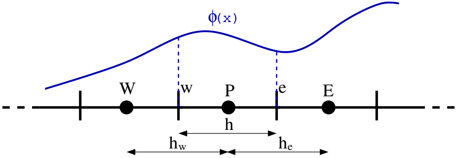

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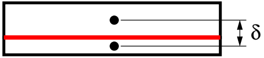

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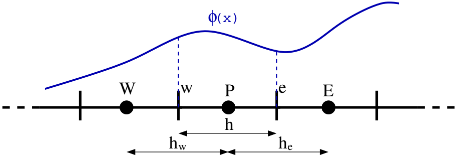

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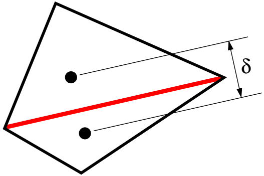

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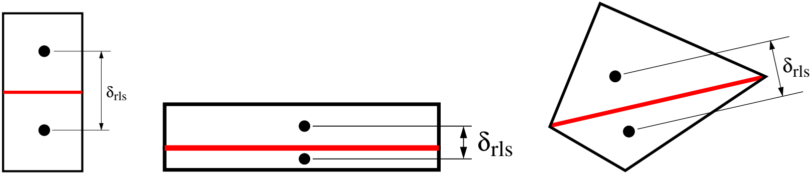
A rational length scale

Properties of new definition, δ_{rls}



A rational length scale

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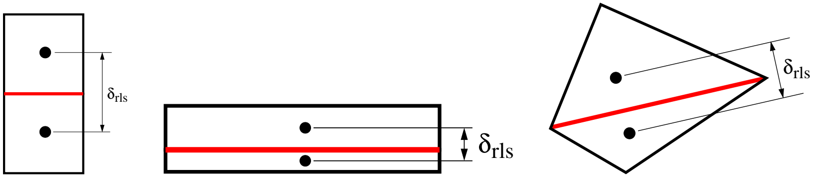
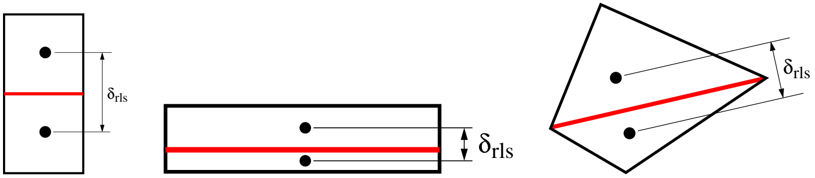


- Locally defined

A rational length scale

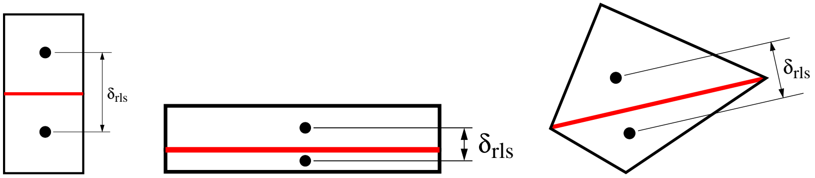
Properties of new definition, δ_{rls}



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

A rational length scale

Properties of new definition, δ_{rls}



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

A rational length scale

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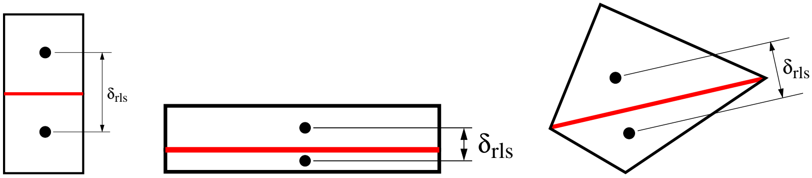

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- Applicable to unstructured grids

A rational length scale

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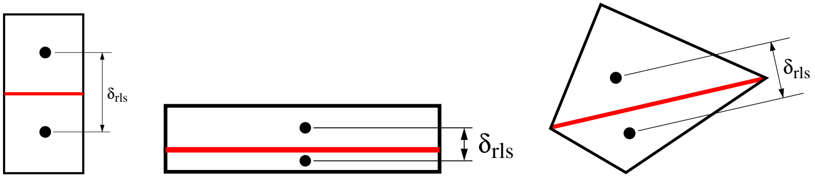
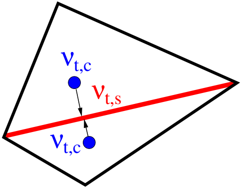


- Locally defined
- Well-bounded: $\Delta x \leqslant \delta_{\mathrm{rls}} \leqslant \Delta z$ (assuming $\Delta x \leqslant \Delta y \leqslant \Delta z$)
- Sensitive to flow orientation, *e.g.* shear layers
- Applicable to unstructured grids
- Easy and cheap

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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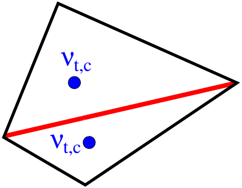

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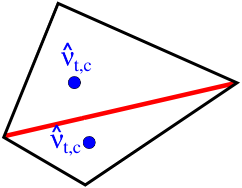
A rational length scale

Implementation and an alternative definition

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

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



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Implementation and an alternative definition

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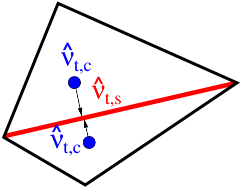

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A rational length scale

Implementation and an alternative definition

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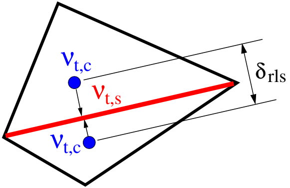

A rational length scale

Implementation and an alternative definition

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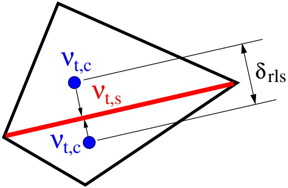

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We can also compute an equivalent filter length, $\tilde{\delta}_{\mathrm{rls}}$, that leads to the same local dissipation

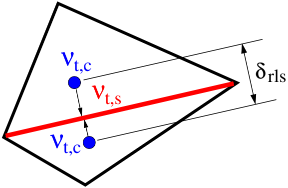
$$\tilde{\delta}^2_{\mathrm{rls}} \hat{\nu}_t \mathsf{G} : \mathsf{G} = \hat{\nu}_t \hat{\mathsf{G}} : \hat{\mathsf{G}}$$

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

A rational length scale

Implementation and an alternative definition

$$\boldsymbol{\nu}_{t,c} \xrightarrow{\text{interpolation}} \boldsymbol{\nu}_{t,s}$$



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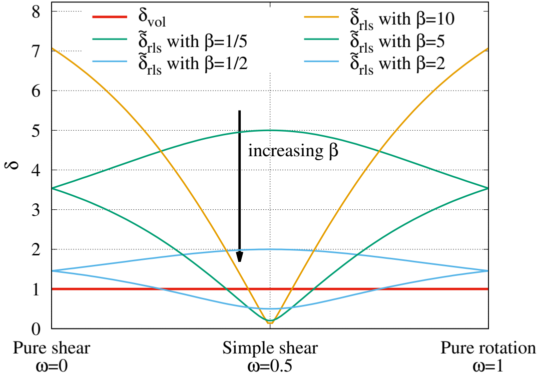
where $\hat{\mathsf{G}} \equiv \mathsf{G}\Delta$ and $\Delta \equiv \mathrm{diag}(\Delta x, \Delta y, \Delta z)$.

A rational length scale

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

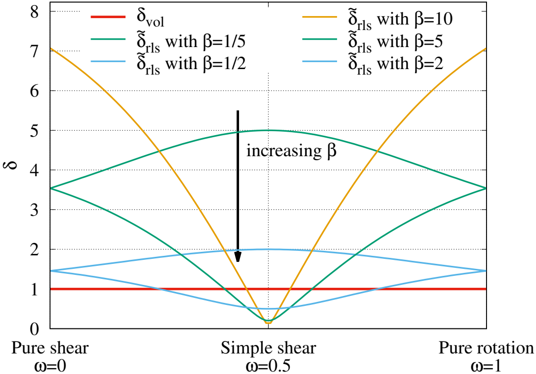
$$\Delta = \begin{pmatrix} \Delta x & 0 \\ 0 & \Delta y \end{pmatrix} \qquad G = \begin{pmatrix} \partial_x u & \partial_y u \\ \partial_y u & \partial_y v \end{pmatrix}$$



A rational length scale

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

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



A rational length scale

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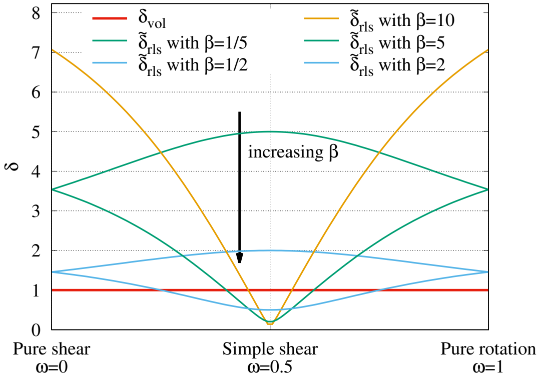
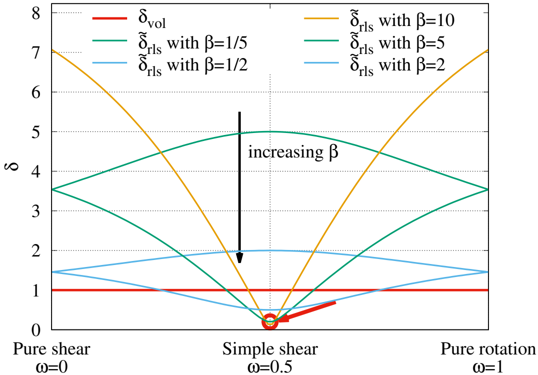
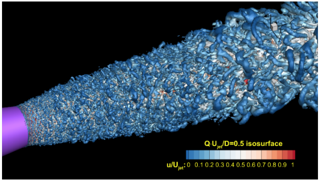


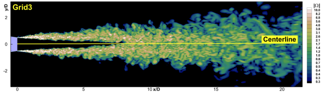
A rational length scale

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

$$\Delta = \begin{pmatrix} \Delta x & 0 \\ 0 & \Delta y \end{pmatrix} = \begin{pmatrix} \beta & 0 \\ 0 & \beta^{-1} \end{pmatrix} \quad G = \begin{pmatrix} \partial_x u & \partial_y u \\ \partial_y u & \partial_y v \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \boxed{\tilde{\delta}_{\text{rls}} = \Delta y}$$



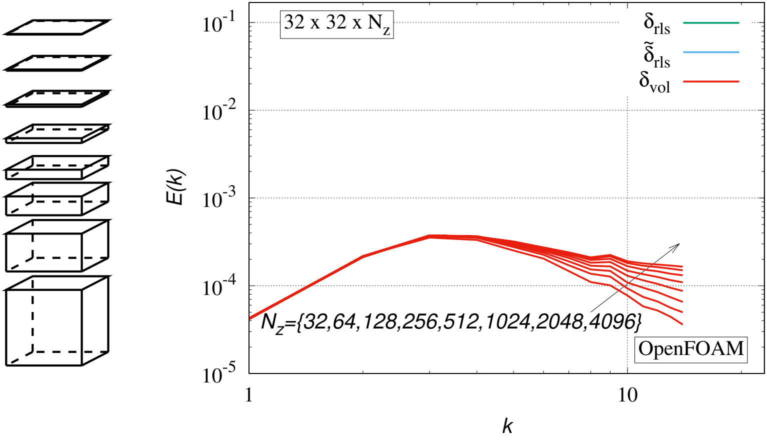




A rational length scale

Isotropic turbulence on anisotropic grids

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



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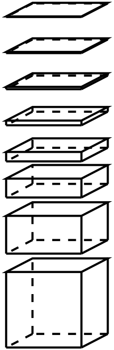

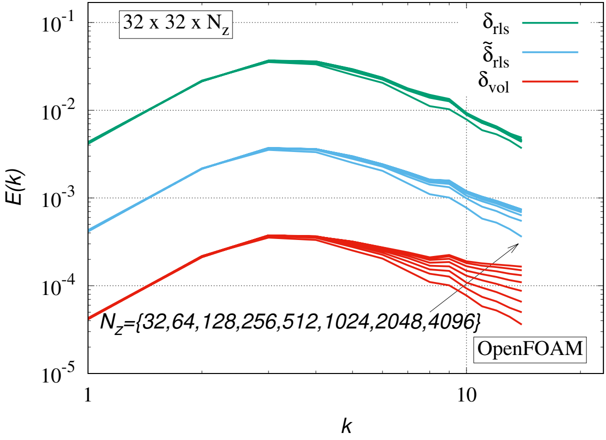

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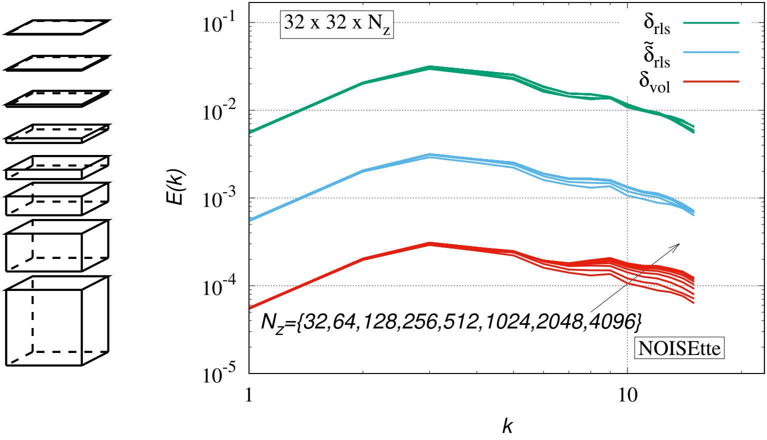

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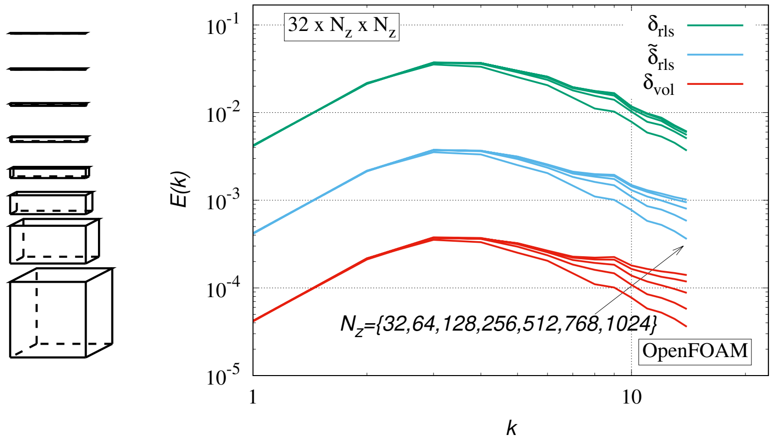
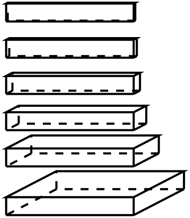
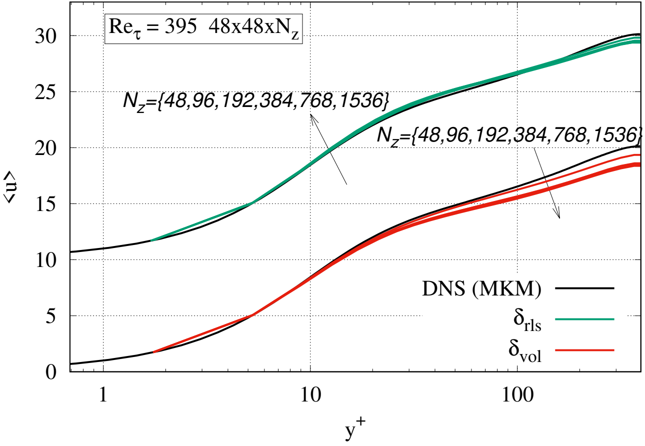


A rational length scale

Turbulent channel flow at $Re_\tau = 395$

Average velocity $48 \times 48 \times N_z$

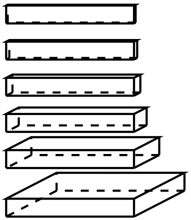


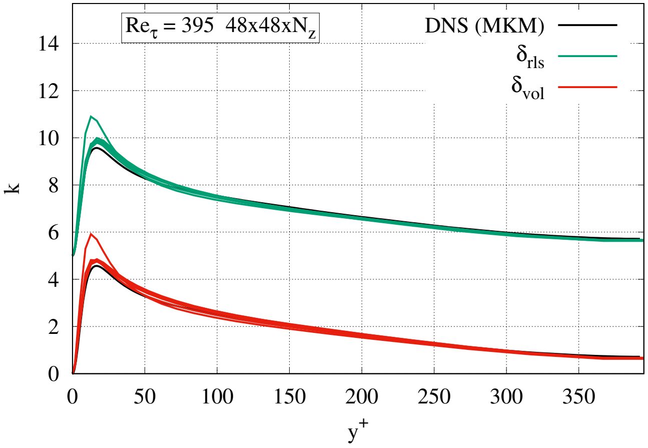


A rational length scale

Turbulent channel flow at $Re_\tau = 395$

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

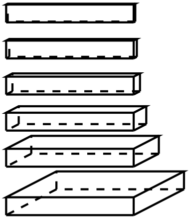


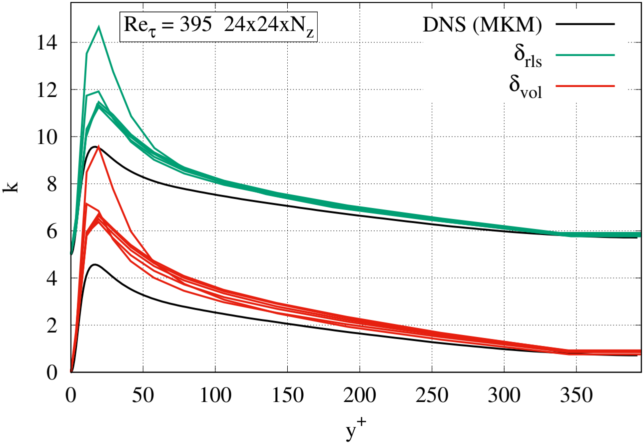


A rational length scale

Turbulent channel flow at $Re_\tau = 395$

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

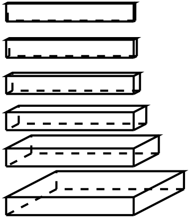


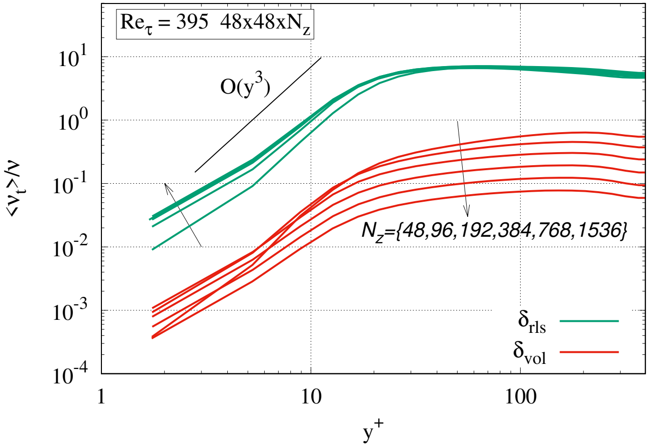


A rational length scale

Turbulent channel flow at $Re_\tau = 395$

Turbulent viscosity $48 \times 48 \times N_z$





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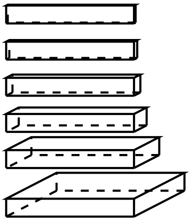
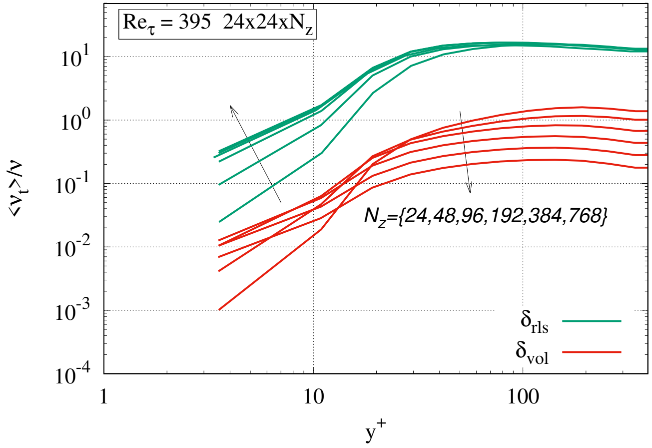
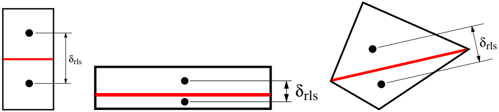




Concluding remarks

- A new definition for δ has been proposed



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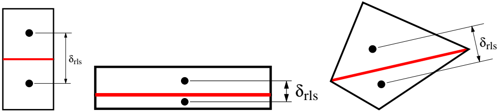

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- It is locally defined, well-bounded, cheap and easy to implement
- Suitable for unstructured grids

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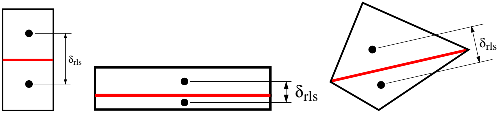

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  - Turbulent channel flow ✓
  - Unstructured grids (on-going)

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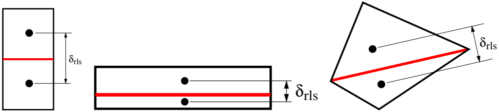

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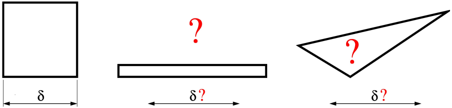

Takeaway message:

- 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

Cite as: Phys. Fluids **37**, 085239 (2025); doi: 10.1063/5.0277423
Submitted: 23 April 2025 · Accepted: 1 August 2025 ·
Published Online: 25 August 2025

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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