



## Interactions between numerical discretization. subgrid modeling and filtering in LES

#### F. Xavier Trias

Heat and Mass Transfer Technological Center, Technical University of Catalonia (UPC)





Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

# Interactions between numerical discretization, subgrid modeling and filtering in LES

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Background





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- 4 A rational length scale for LES
- Conclusions

## Contents

Background

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- 2 Motivation
- Revisiting FVM
- 4 A rational length scale for LES
- 6 Conclusions

### Professional

Background

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- Current position (since 2024): Full Professor at UPC
- Previous positions: PostDoc at University of Groningen (2007-2009) and UPC (2010-2013), Ramón y Cajal Senior Researcher at UPC (2013-2018) and Associate Professor (2018-2023).
- My research focus is on fluid mechanics, turbulence modeling, physics and numerics of complex flows, applied mathematics and numerical methods.
- Some numbers: 58 papers, 190 conferences, 12 PhD's+5 (on-going)
- Stays and collaborations: Groningen (Netherlands), UCLA, KIAM (Russian Academy of Sciences), Stanford, Tsinghua (China), TokioTech (Japan), Napoli (Italy), CWI (Netherlands),...
- More info: www.fxtrias.com

## About myself...

... and more personal stuff

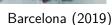
- My complete name: Francesc Xavier Trias Miquel
- Born in Barcelona
- My mother tongue is Catalan. I also speak Spanish at native level.
- Hobbies? I like my work but also sports. Most practiced ones are running and football:





Groningen (2009?)





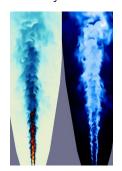


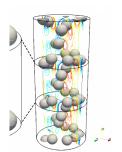
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## The CTTC research group

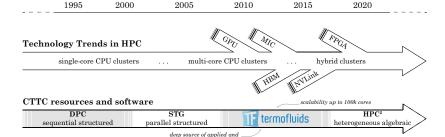
Heat and Mass Transfer Technological Center (Catalan: Centre Tecnològic de Transferència de Calor) has more than 30 years experience on CFD:

- Fundamental research on numerical methods, fluid dynamics and heat and mass transfer phenomena.
- Applied research on thermal and fluid dynamic optimization of thermal system and equipment.









fundamental research



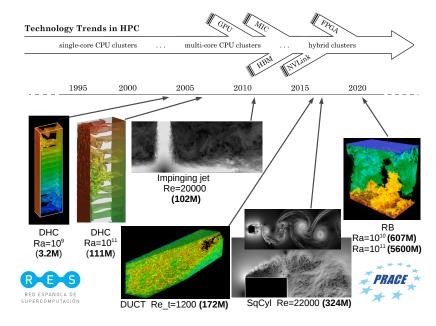
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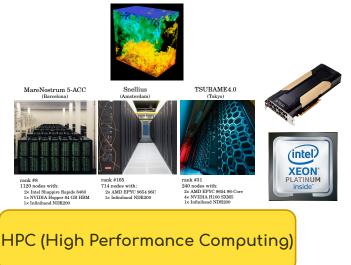
## General motivation: (very) large-scale DNS/LES





DNS

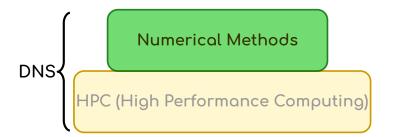
## General motivation: (very) large-scale DNS/LES



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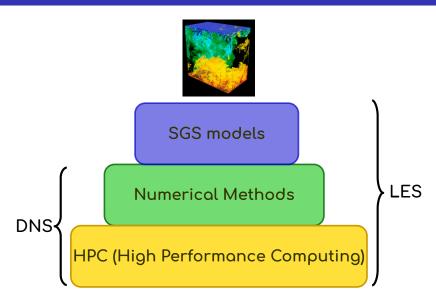
## How to properly discretize NS?



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

How to properly model SGS? SGS models **LFS** Numerical Methods **DNS** HPC (High Performance Computing)

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



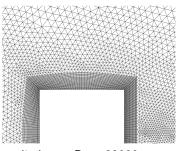
### Contents

- Motivation

#### Motivation

#### Research question #1:

• What are we indeed solving with finite volume method?

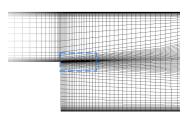


 $\mathsf{DNS}^1$  of the turbulent flow around a square cylinder at Re = 22000

<sup>&</sup>lt;sup>1</sup>F.X.Trias, A.Gorobets, A.Oliva. *Turbulent flow around a square cylinder at Reynolds number 22000: a DNS study*, **Computers&Fluids**, 123:87-98, 2015.

## Research question #1:

• What are we indeed solving with finite volume method?



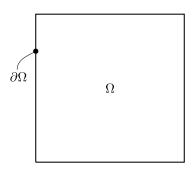
DNS<sup>2</sup> of backward-facing step at  $Re_{\tau} = 395$  and expansion ratio 2

<sup>&</sup>lt;sup>2</sup>A.Pont-Vílchez, F.X.Trias, A.Gorobets, A.Oliva. DNS of Backward-Facing Step flow at  $Re_{\tau} = 395$  and expansion ratio 2. Journal of Fluid Mechanics, 863:341-363, 2019.

#### Motivation

#### Research question #2:

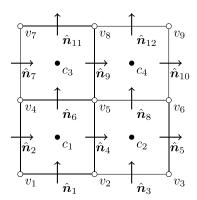
• What are we interpolating? What is the correct interpretation?



#### Motivation

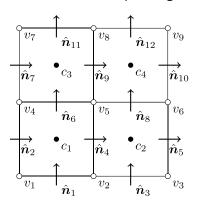
#### Research question #2:

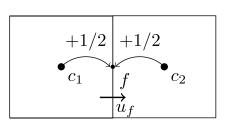
• What are we interpolating? What is the correct interpretation?



#### Research question #2:

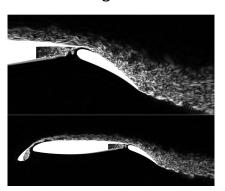
• What are we interpolating? What is the correct interpretation?

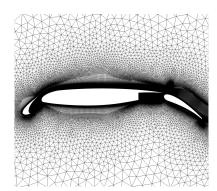




## Research question #3:

• Can we developed high-order symmetry-preserving schemes for unstructured grids?

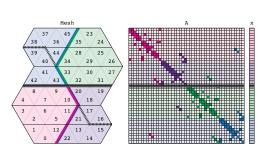


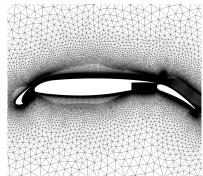


#### Motivation

#### Research question #3:

 Can we developed high-order symmetry-preserving schemes for unstructured grids? And, therefore, get better performance





## Reminder: symmetry-preserving discretization

#### Continuous

$$\frac{\partial \mathbf{u}}{\partial t} + C(\mathbf{u}, \mathbf{u}) = \nu \nabla^2 \mathbf{u} - \nabla \mathbf{p}$$
$$\nabla \cdot \mathbf{u} = 0$$

Continuous

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{C}(\mathbf{u}, \mathbf{u}) = \nu \nabla^2 \mathbf{u} - \nabla \mathbf{p}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{C}(\boldsymbol{u}, \boldsymbol{u}) = \nu \nabla^2 \boldsymbol{u} - \nabla p \qquad \Omega \frac{d\boldsymbol{u}_h}{dt} + \boldsymbol{C}(\boldsymbol{u}_h) \boldsymbol{u}_h = \boldsymbol{D} \boldsymbol{u}_h - \boldsymbol{G}_h \boldsymbol{p}_h$$

$$\nabla \cdot \boldsymbol{u} = 0 \qquad \qquad \boldsymbol{M} \boldsymbol{u}_h = \boldsymbol{0}_h$$

## Reminder: symmetry-preserving discretization

#### Continuous

$$\frac{\partial \mathbf{u}}{\partial t} + C(\mathbf{u}, \mathbf{u}) = \nu \nabla^2 \mathbf{u} - \nabla p$$
$$\nabla \cdot \mathbf{u} = 0$$

$$(\mathbf{a}, \mathbf{b}) = \int_{\Omega} \mathbf{a} \mathbf{b} d\Omega$$

$$\Omega \frac{d\mathbf{u}_h}{dt} + C(\mathbf{u}_h) \mathbf{u}_h = \mathbf{D}\mathbf{u}_h - \mathbf{G}_h \mathbf{p}_h$$
$$\mathbf{M}\mathbf{u}_h = \mathbf{0}_h$$

$$(\boldsymbol{a}_h, \boldsymbol{b}_h)_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$$

## Reminder: symmetry-preserving discretization

Continuous

$$\frac{\partial \mathbf{u}}{\partial t} + C(\mathbf{u}, \mathbf{u}) = \nu \nabla^2 \mathbf{u} - \nabla p$$
$$\nabla \cdot \mathbf{u} = 0$$

$$(\mathbf{a}, \mathbf{b}) = \int_{\Omega} \mathbf{a} \mathbf{b} d\Omega$$

$$(C(\mathbf{u},\phi_1),\phi_2) = -(C(\mathbf{u},\phi_2),\phi_1)$$

$$\Omega \frac{d\boldsymbol{u}_h}{dt} + C(\boldsymbol{u}_h) \boldsymbol{u}_h = D\boldsymbol{u}_h - G_h \boldsymbol{p}_h$$

$$M\boldsymbol{u}_h = \boldsymbol{0}_h$$

$$(\boldsymbol{a}_h, \boldsymbol{b}_h)_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$$

$$C\left(\boldsymbol{u}_{h}\right)=-C^{T}\left(\boldsymbol{u}_{h}\right)$$

## Reminder: symmetry-preserving discretization

#### Continuous

$$\frac{\partial \mathbf{u}}{\partial t} + C(\mathbf{u}, \mathbf{u}) = \nu \nabla^2 \mathbf{u} - \nabla p$$
$$\nabla \cdot \mathbf{u} = 0$$

$$(\boldsymbol{a}, \boldsymbol{b}) = \int_{\Omega} \boldsymbol{a} \boldsymbol{b} d\Omega$$

$$(C(\mathbf{u}, \phi_1), \phi_2) = -(C(\mathbf{u}, \phi_2), \phi_1)$$
$$(\nabla \cdot \mathbf{a}, \phi) = -(\mathbf{a}, \nabla \phi)$$

$$\Omega \frac{d\boldsymbol{u}_h}{dt} + C(\boldsymbol{u}_h) \boldsymbol{u}_h = D\boldsymbol{u}_h - G_h \boldsymbol{p}_h$$
$$M\boldsymbol{u}_h = \boldsymbol{0}_h$$

$$(\boldsymbol{a}_h, \boldsymbol{b}_h)_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$$

$$C(\boldsymbol{u}_h) = -C^T(\boldsymbol{u}_h)$$
$$\Omega G_h = -M^T$$

## Reminder: symmetry-preserving discretization

#### Continuous

$$\frac{\partial \mathbf{u}}{\partial t} + C(\mathbf{u}, \mathbf{u}) = \nu \nabla^2 \mathbf{u} - \nabla p$$
$$\nabla \cdot \mathbf{u} = 0$$

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$$(\nabla \cdot \mathbf{a}, \phi) = -(\mathbf{a}, \nabla \phi)$$
$$(\nabla^2 \mathbf{a}, \mathbf{b}) = (\mathbf{a}, \nabla^2 \mathbf{b})$$

$$\Omega \frac{d\mathbf{u}_h}{dt} + \mathbf{C}(\mathbf{u}_h) \mathbf{u}_h = \mathbf{D}\mathbf{u}_h - \mathbf{G}_h \mathbf{p}_h$$
$$\mathbf{M}\mathbf{u}_h = \mathbf{0}_h$$

$$(\boldsymbol{a}_h, \boldsymbol{b}_h)_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$$

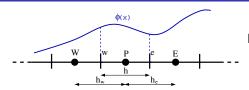
$$C(\mathbf{u}_h) = -C^T(\mathbf{u}_h)$$

$$\Omega G_h = -M^T$$

$$D = D^T \quad def - C^T(\mathbf{u}_h)$$

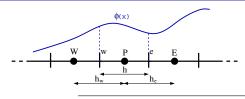
## Contents

- Revisiting FVM



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

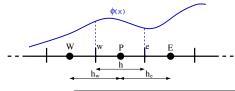
$$\partial_x \overline{\phi}|_e = \overline{\partial_x \phi}|_e = (\phi_E - \phi_P)/h_e$$



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

$$\partial_{\mathsf{x}}\overline{\phi}|_{\mathsf{e}} = \overline{\partial_{\mathsf{x}}\phi}|_{\mathsf{e}} = (\phi_{\mathsf{E}} - \phi_{\mathsf{P}})/h_{\mathsf{e}}$$

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



Box filter:

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

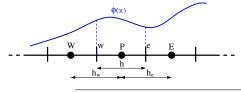
$$\partial_{\mathsf{x}}\overline{\phi}|_{\mathsf{e}} = \overline{\partial_{\mathsf{x}}\phi}|_{\mathsf{e}} = (\phi_{\mathsf{E}} - \phi_{\mathsf{P}})/h_{\mathsf{e}}$$

$$\frac{\partial \phi}{\partial t} + \frac{\partial (\mathbf{u}\phi)}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2} \quad -$$

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

Exact FVM eq!

Background



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

$$\partial_{\mathbf{x}}\overline{\phi}|_{\mathbf{e}} = \overline{\partial_{\mathbf{x}}\phi}|_{\mathbf{e}} = (\phi_{\mathbf{E}} - \phi_{\mathbf{P}})/h_{\mathbf{e}}$$

$$\frac{\partial \phi}{\partial t} + \frac{\partial (\mathbf{u}\phi)}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2} \longrightarrow \boxed{\frac{\partial \overline{\phi}}{\partial t} + \overline{\frac{\partial (\mathbf{u}\phi)}{\partial x}} = \nu \overline{\frac{\partial^2 \phi}{\partial x^2}}} \text{ Exact FVM eq!}$$

$$h\frac{\partial\overline{\phi}_{P}}{\partial t} + (\mathbf{u}\phi)_{e} - (\mathbf{u}\phi)_{w} = \nu \left( \frac{\partial\phi}{\partial x} \Big|_{e} - \frac{\partial\phi}{\partial x} \Big|_{w} \right)$$



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

$$\partial_{\mathsf{x}}\overline{\phi}|_{\mathsf{e}} = \overline{\partial_{\mathsf{x}}\phi}|_{\mathsf{e}} = (\phi_{\mathsf{E}} - \phi_{\mathsf{P}})/h_{\mathsf{e}}$$

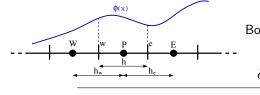
$$\frac{\partial \phi}{\partial t} + \frac{\partial (\mathbf{u}\phi)}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2} \longrightarrow \left| \frac{\partial \overline{\phi}}{\partial t} + \frac{\overline{\partial (\mathbf{u}\phi)}}{\partial x} \right| = \nu \frac{\overline{\partial^2 \phi}}{\partial x^2} \quad \text{Exact FVM eq!}$$

$$h\frac{\partial \overline{\phi}_{P}}{\partial t} + (\mathbf{u}\phi)_{e} - (\mathbf{u}\phi)_{w} = \nu \left( \frac{\partial \phi}{\partial x} \Big|_{e} - \frac{\partial \phi}{\partial x} \Big|_{w} \right)$$

$$\frac{1}{\partial t} + (\mathbf{u}\phi)_{e} - (\mathbf{u}\phi)_{w} - \nu \left( \frac{\partial}{\partial x} \Big|_{e} - \frac{\partial}{\partial x} \Big|_{w} \right)$$

$$\int \partial \overline{\phi}_{P}$$

$$\boxed{\frac{\partial \overline{\phi}}{\partial t} + } =$$



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

$$\partial_{\mathsf{x}}\overline{\phi}|_{\mathsf{e}} = \overline{\partial_{\mathsf{x}}\phi}|_{\mathsf{e}} = (\phi_{\mathsf{E}} - \phi_{\mathsf{P}})/h_{\mathsf{e}}$$

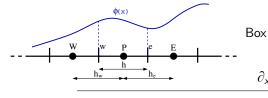
$$\frac{\partial \phi}{\partial t} + \frac{\partial (\mathbf{u}\phi)}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2} \longrightarrow \left| \frac{\partial \overline{\phi}}{\partial t} + \frac{\overline{\partial (\mathbf{u}\phi)}}{\partial x} \right| = \nu \frac{\overline{\partial^2 \phi}}{\partial x^2} \quad \text{Exact FVM eq!}$$

$$h\frac{\partial\overline{\phi}_{P}}{\partial t} + (\mathbf{u}\phi)_{e} - (\mathbf{u}\phi)_{w} = \nu \left( \frac{\partial\phi}{\partial x} \Big|_{e} - \frac{\partial\phi}{\partial x} \Big|_{w} \right)$$
$$= \nu \left( \frac{\overline{\phi}_{E} - \overline{\phi}_{P}}{h_{e}} - \frac{\overline{\phi}_{P} - \overline{\phi}_{W}}{h_{w}} \right)$$

$$\boxed{\frac{\partial \overline{\phi}}{\partial t} + = \nu \frac{\overline{\frac{\partial^2 \overline{\overline{\phi}}}{\overline{\phi}}}}{\partial x^2}}$$

# Revisiting FVM

Background



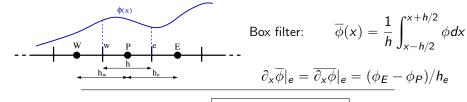
$$\overline{\phi}(x) = \frac{1}{h} \int_{x-h/2}^{x+h/2} \phi dx$$

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

$$\frac{\partial \phi}{\partial t} + \frac{\partial (\mathbf{u}\phi)}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2} \longrightarrow \left| \frac{\partial \overline{\phi}}{\partial t} + \frac{\overline{\partial (\mathbf{u}\phi)}}{\partial x} \right| = \nu \frac{\overline{\partial^2 \phi}}{\overline{\partial x^2}}$$
 Exact FVM eq!

$$\begin{split} h\frac{\partial\overline{\phi}_{P}}{\partial t} + (\textbf{\textit{u}}\phi)_{e} - (\textbf{\textit{u}}\phi)_{w} &= \nu \left( \left. \frac{\partial\phi}{\partial x} \right|_{e} - \left. \frac{\partial\phi}{\partial x} \right|_{w} \right) \\ h\frac{\partial\overline{\phi}_{P}}{\partial t} + \textbf{\textit{u}}_{e}\frac{\overline{\phi}_{P} + \overline{\phi}_{E}}{2} - \textbf{\textit{u}}_{w}\frac{\overline{\phi}_{W} + \overline{\phi}_{P}}{2} &= \nu \left( \frac{\overline{\phi}_{E} - \overline{\phi}_{P}}{h_{e}} - \frac{\overline{\phi}_{P} - \overline{\phi}_{W}}{h_{w}} \right) \end{split}$$

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



$$\frac{\partial \phi}{\partial t} + \frac{\partial (\mathbf{u}\phi)}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2} \longrightarrow \left| \frac{\partial \overline{\phi}}{\partial t} + \overline{\frac{\partial (\mathbf{u}\phi)}{\partial x}} \right| = \nu \frac{\overline{\partial^2 \phi}}{\overline{\partial x^2}} \quad \text{Exact FVM eq!}$$

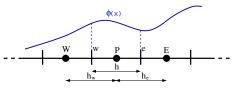
$$\begin{split} h\frac{\partial\overline{\phi}_{P}}{\partial t} + (\textbf{\textit{u}}\phi)_{e} - (\textbf{\textit{u}}\phi)_{w} &= \nu \left( \left. \frac{\partial\phi}{\partial x} \right|_{e} - \left. \frac{\partial\phi}{\partial x} \right|_{w} \right) \\ h\frac{\partial\overline{\phi}_{P}}{\partial t} + \textbf{\textit{u}}_{e} \frac{\overline{\phi}_{P} + \overline{\phi}_{E}}{2} - \textbf{\textit{u}}_{w} \frac{\overline{\phi}_{W} + \overline{\phi}_{P}}{2} &= \nu \left( \frac{\overline{\phi}_{E} - \overline{\phi}_{P}}{h_{e}} - \frac{\overline{\phi}_{P} - \overline{\phi}_{W}}{h_{w}} \right) \end{split}$$

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

 $\frac{\partial \overline{\phi}}{\partial z} + \frac{\partial (\mathbf{u} \overline{\phi})}{\partial z} = \nu \frac{\partial^2 \overline{\phi}}{\partial z^2} \bigg| \qquad \text{where } \widetilde{\phi}_e = \frac{\overline{\phi}_P + \overline{\phi}_E}{2} = \overline{\phi}_e + \mathcal{O}(h^2)$ 

#### Revisiting FVM

Background



Box filter:

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

$$\partial_{\mathsf{x}}\overline{\phi}|_{\mathsf{e}} = \overline{\partial_{\mathsf{x}}\phi}|_{\mathsf{e}} = (\phi_{\mathsf{E}} - \phi_{\mathsf{P}})/h_{\mathsf{e}}$$

In summary (assuming that u is known):

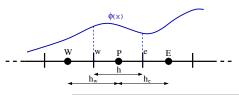
$$\frac{\partial \overline{\phi}}{\partial t} + \frac{\overline{\partial (\mathbf{u}\phi)}}{\partial x} = \nu \frac{\overline{\partial^2 \phi}}{\partial x^2}$$

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

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

#### Revisiting FVM

Background



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

$$\partial_{\mathsf{x}}\overline{\phi}|_{\mathsf{e}} = \overline{\partial_{\mathsf{x}}\phi}|_{\mathsf{e}} = (\phi_{\mathsf{E}} - \phi_{\mathsf{P}})/h_{\mathsf{e}}$$

In summary (assuming that u is known):

$$\frac{\partial \overline{\phi}}{\partial t} + \overline{\frac{\partial (\mathbf{u}\phi)}{\partial x}} = \nu \overline{\frac{\partial^2 \phi}{\partial x^2}} \quad \longrightarrow \quad \overline{\left(\frac{\partial \varphi}{\partial t} + \frac{\partial (\mathbf{u}\varphi)}{\partial x} = \nu \frac{\partial^2 \varphi}{\partial x^2}\right)} \quad \text{Exact FVM eq!}$$

$$\boxed{\frac{\partial \varphi}{\partial t} + \frac{\partial (\mathbf{u}\varphi)}{\partial x} = \nu \frac{\partial^2 \varphi}{\partial x^2}}$$

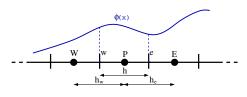
Instead, we are solving (in a  $2^{nd}$ -order symmetry-preserving discretization):

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

$$\boxed{\frac{\partial \varphi}{\partial t} + \frac{\overline{\partial (\mathbf{u}\overline{\varphi})}}{\partial x} = \nu \frac{\overline{\partial^2 \overline{\varphi}}}{\partial x^2}}$$

Approx FVM eq!

#### Towards high-order via deconvolution



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

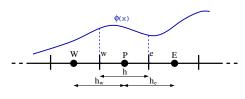
$$\partial_{\mathsf{x}}\overline{\phi}|_{\mathsf{e}} = \overline{\partial_{\mathsf{x}}\phi}|_{\mathsf{e}} = (\phi_{\mathsf{E}} - \phi_{\mathsf{P}})/h_{\mathsf{e}}$$

Hence, the standard 2<sup>nd</sup>-order symmetry-preserving FVM can be viewed as

$$\frac{\partial^2 \varphi}{\partial x^2} \approx \frac{\partial^2 \overline{\varphi}}{\partial x^2} + \mathcal{O}(h^2)$$
 where  $\frac{\partial^2 \overline{\varphi}}{\partial x^2} = \frac{\varphi_E - 2\varphi_P + \varphi_W}{h^2}$ 

$$\frac{\partial^2 \overline{\varphi}}{\partial x^2} = \frac{\varphi_E - 2\varphi_P + \varphi_W}{h^2}$$

#### Towards high-order via deconvolution



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

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

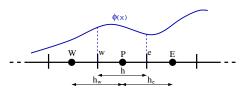
Hence, the standard  $2^{nd}$ -order symmetry-preserving FVM can be viewed as

$$\frac{\partial^2 \varphi}{\partial x^2} \approx \frac{\overline{\partial^2 \overline{\varphi}}}{\overline{\partial x^2}} + \mathcal{O}(h^2)$$
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Recalling that  $\phi = \overline{\phi} + \phi'$ 

$$\frac{\partial^2 \varphi}{\partial x^2} = \frac{\overline{\partial^2 \overline{\varphi}}}{\partial x^2} + \overline{\frac{\partial^2 \varphi'}{\partial x^2}} + \left(\frac{\partial^2 \overline{\varphi}}{\partial x^2}\right)' + \left(\frac{\partial^2 \varphi'}{\partial x^2}\right)'$$

# Towards high-order via deconvolution



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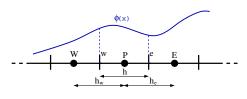
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Recalling that  $\phi = \overline{\phi} + \phi'$  and  $\phi'_P \approx -\frac{1}{24}(\varphi_E - 2\varphi_P + \varphi_W) + \mathcal{O}(h^2)$ 

$$\frac{\partial^2 \varphi}{\partial x^2} = \frac{\overline{\partial^2 \overline{\varphi}}}{\overline{\partial x^2}} + \frac{\overline{\partial^2 \varphi'}}{\overline{\partial x^2}} + \left(\frac{\partial^2 \overline{\varphi}}{\partial x^2}\right)' + \mathcal{O}(h^4)$$

# Towards high-order via deconvolution



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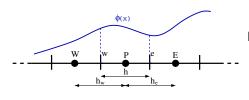
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$$\frac{\partial^2 \varphi}{\partial x^2} = \frac{\varphi_F - 2\varphi_P + \varphi_W}{2} - \varphi_{FF} + 4\varphi_{FF}$$

$$\frac{\partial^2 \varphi}{\partial x^2} \approx \frac{\varphi_E - 2\varphi_P + \varphi_W}{h^2} + 2\frac{-\varphi_{EE} + 4\varphi_E - 6\varphi_P + 4\varphi_W - \varphi_{WW}}{24h^2}$$

# Towards high-order via deconvolution



Box filter: 
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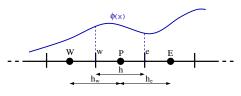
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$$\frac{\partial^{2} \varphi}{\partial x^{2}} \approx \frac{-\varphi_{EE} + 16\varphi_{E} - 30\varphi_{P} + 16\varphi_{W} - \varphi_{WW}}{12h^{2}} + \mathcal{O}(h^{4})$$

#### Towards high-order via deconvolution



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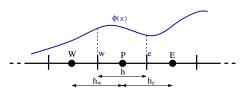
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In summary, in 1D we have:

$$\frac{\partial^{2} \varphi}{\partial x^{2}} = \frac{\overline{\partial^{2} \overline{\varphi}}}{\partial x^{2}} + \frac{\overline{\partial^{2} \varphi'}}{\partial x^{2}} + \left(\frac{\partial^{2} \overline{\varphi}}{\partial x^{2}}\right)' + \mathcal{O}(h^{4})$$

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This can be extended to 2D/3D (notice that  $\varphi' = -\frac{h^2}{24}\nabla^2\varphi + \mathcal{O}(h^4)$ )

$$\boxed{ \nabla^2 \varphi = \overline{\nabla^2 \overline{\varphi}} + \overline{\nabla^2 \varphi'} + (\nabla^2 \overline{\varphi})' + \mathcal{O}(\mathit{h}^4) }$$

#### Contents

- 4 A rational length scale for LES

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# Subgrid characteristic length for LES: state of the art

$$\partial_{t}\overline{\boldsymbol{u}} + (\overline{\boldsymbol{u}} \cdot \nabla)\overline{\boldsymbol{u}} = \nabla^{2}\overline{\boldsymbol{u}} - \nabla\overline{\boldsymbol{p}} - \nabla \cdot \boldsymbol{\tau}(\overline{\boldsymbol{u}}) ; \quad \nabla \cdot \overline{\boldsymbol{u}} = 0$$
eddy-viscosity  $\longrightarrow \boldsymbol{\tau} (\overline{\boldsymbol{u}}) = -2\nu_{t}S(\overline{\boldsymbol{u}})$ 

<sup>&</sup>lt;sup>3</sup>F.X.Trias, D.Folch, A.Gorobets, A.Oliva. Building proper invariants for eddy-viscosity subgrid-scale models, Physics of Fluids, 27: 065103, 2015.

<sup>&</sup>lt;sup>4</sup>M.Silvis, R.Remmerswaal, R.Verstappen, **Physics of Fluids**, 29: 015105, 2017.

$$\begin{split} \partial_t \overline{\boldsymbol{u}} + (\overline{\boldsymbol{u}} \cdot \nabla) \overline{\boldsymbol{u}} &= \nabla^2 \overline{\boldsymbol{u}} - \nabla \overline{\boldsymbol{p}} - \nabla \cdot \boldsymbol{\tau}(\overline{\boldsymbol{u}}) \; ; \quad \nabla \cdot \overline{\boldsymbol{u}} = 0 \\ \text{eddy-viscosity} &\longrightarrow \boldsymbol{\tau} \; (\overline{\boldsymbol{u}}) = -2\nu_t S(\overline{\boldsymbol{u}}) \end{split}$$

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$$\nu_t = (C_m \delta)^2 D_m(\overline{\boldsymbol{u}})$$

 $D_m(\overline{u}) \longrightarrow \text{Smagorinsky (1963), WALE (1999), Vreman (2004),}$ QR-model (2011),  $\sigma$ -model (2011), S3PQR<sup>3</sup> (2015), vortex-stretching-based model<sup>4</sup> (2017)

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#### Subgrid characteristic length for LES: state of the art

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

$$\begin{array}{|c|c|}\hline \delta_{\rm vol} = (\Delta x \Delta y \Delta z)^{1/3} & \longleftarrow \text{Deardorff (1970)}\\ \delta_{\rm Sco} = f(\textit{a}_1,\textit{a}_2)\delta_{\rm vol}, & \delta_{\textit{L}^2} = \sqrt{(\Delta x^2 + \Delta y^2 + \Delta z^2)/3} \end{array}$$

#### Subgrid characteristic length for LES: state of the art

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

$$\begin{split} \delta_{\mathrm{vol}} &= (\Delta x \Delta y \Delta z)^{1/3} \\ &\iff \text{Deardorff (1970)} \\ \delta_{\mathrm{Sco}} &= f(a_1, a_2) \delta_{\mathrm{vol}}, \qquad \delta_{L^2} &= \sqrt{(\Delta x^2 + \Delta y^2 + \Delta z^2)/3} \\ \delta_{\mathrm{lsq}} &= \sqrt{\frac{\hat{\mathsf{G}}\hat{\mathsf{G}}^T : \mathsf{G}\mathsf{G}^T}{\mathsf{G}\mathsf{G}^T : \mathsf{G}\mathsf{G}^T}} &\iff \text{Trias et al. (2017)} \end{split}$$

# Subgrid characteristic length for LES: state of the art

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

• In the context of DES:

$$\delta_{\mathsf{max}} = \mathsf{max}(\Delta x, \Delta y, \Delta z)$$
  $\longleftarrow$  Sparlart et al. (1997)

Flow-dependent definitions

#### Research question #4:

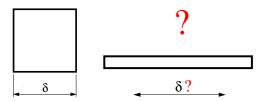
• Can we establish a **simple**, **robust**, and **easily implementable** definition of  $\delta$  for any type of grid that minimizes the impact of mesh anisotropies on the performance of subgrid-scale models?



#### Research question #4:

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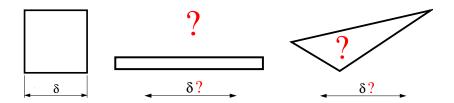
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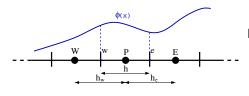
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# A rational length scale for LES

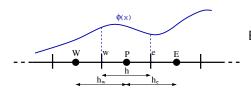


Box filter: 
$$\overline{\phi}(x) = \frac{1}{h} \int_{x-h/2}^{x+h/2} \phi dx$$

$$\partial_{\mathsf{x}}\overline{\phi} = \overline{\partial_{\mathsf{x}}\phi} = (\phi_{\mathsf{e}} - \phi_{\mathsf{w}})/h$$

**Remark** #1: the actual filter length,  $\delta$ , 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

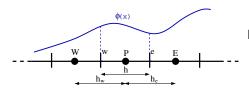


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The diffusive term in a FVM framework is approximated as follows

$$\left. \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \phi}{\partial x} \right) \right|_{P} \approx \left. \frac{1}{h} \left( \Gamma \frac{\partial \phi}{\partial x} \right|_{e} - \left. \Gamma \frac{\partial \phi}{\partial x} \right|_{w} \right) = \left. \overline{\frac{\partial}{\partial x} \left( \Gamma \frac{\partial \phi}{\partial x} \right)} \right|_{P}$$

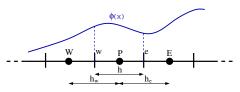


Box filter:  $\overline{\phi}(x) = \frac{1}{h} \int_{-\infty}^{x+h/2} \phi dx$ 

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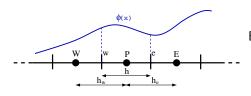


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A rational length scale for LES

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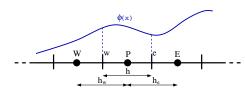
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Remark #2: two filtering operations are performed when computing the diffusive term:

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

$$\left. \frac{\partial}{\partial x} \left( \overline{\Gamma} \frac{\overline{\partial \phi}}{\overline{\partial x}} \right) \right|_{E}$$

# A rational length scale for LES



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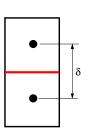
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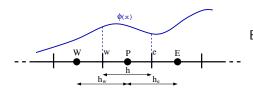
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A rational length scale for LES

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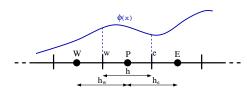
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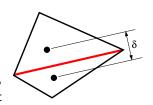
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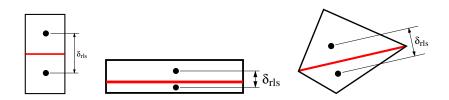
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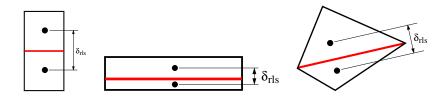
Both filtering operators share the same filter length,  $\delta$ ; namely, the distance between the nodes adjacent to the corresponding face.



Properties of new definition,  $\delta_{\rm rls}$ 

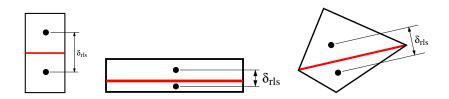


Properties of new definition,  $\delta_{\rm rls}$ 



Locally defined

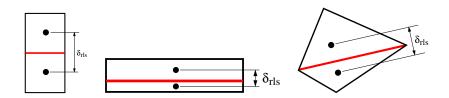
Properties of new definition,  $\delta_{\rm rls}$ 



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

Properties of new definition,  $\delta_{\rm rls}$ 

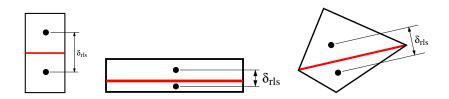
Background



- Locally defined
- Well-bounded:  $\Delta x \leq \delta_{\rm rls} \leq \Delta z$  (assuming  $\Delta x \leq \Delta y \leq \Delta z$ )
- Sensitive to flow orientation, e.g. shear layers

Properties of new definition,  $\delta_{\rm rls}$ 

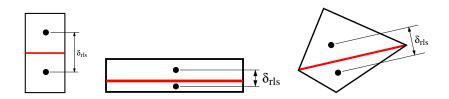
Background



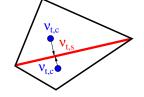
- Locally defined
- Well-bounded:  $\Delta x \leq \delta_{\rm rls} \leq \Delta z$  (assuming  $\Delta x \leq \Delta y \leq \Delta z$ )
- Sensitive to flow orientation, e.g. shear layers
- Applicable to unstructured grids

Properties of new definition,  $\delta_{\rm rls}$ 

Background

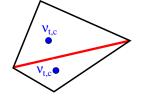


- Locally defined
- Well-bounded:  $\Delta x \leq \delta_{\rm rls} \leq \Delta z$  (assuming  $\Delta x \leq \Delta y \leq \Delta z$ )
- Sensitive to flow orientation, e.g. shear layers
- Applicable to unstructured grids
- Easy and cheap



$$u_{t,c} \xrightarrow{\cdots} \hat{\nu}_{t,c} \xrightarrow{} \hat{\nu}_{t,s} \xrightarrow{\cdots} \nu_{t,s}$$

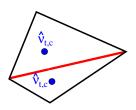
Implementation and an alternative definition



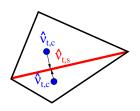
A rational length scale for LES

$$u_{t,c} \xrightarrow{} \hat{\nu}_{t,c} \xrightarrow{} \hat{\nu}_{t,s} \xrightarrow{} \nu_{t,s}$$

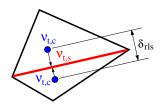
$${\color{red} \boldsymbol{\nu}_{t,c}} \stackrel{1/\delta_{vol}^2}{---} \hat{\boldsymbol{\nu}}_{t,c} \stackrel{1}{----} \hat{\boldsymbol{\nu}}_{t,s} \stackrel{1}{----} \boldsymbol{\nu}_{t,s}$$



$$oldsymbol{
u}_{t,c} \stackrel{1/\delta_{vol}^2}{----} \hat{oldsymbol{
u}}_{t,c} \stackrel{ ext{interpolation}}{\longrightarrow} \hat{oldsymbol{
u}}_{t,s} \stackrel{\dots}{\longrightarrow} oldsymbol{
u}_{t,s}$$



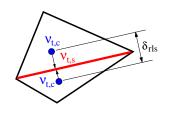
$$\boldsymbol{\nu}_{t,c} \xrightarrow{1/\delta_{vol}^2} \hat{\boldsymbol{\nu}}_{t,c} \xrightarrow{\text{interpolation}} \hat{\boldsymbol{\nu}}_{t,s} \xrightarrow{\delta_{rls}^2} \boldsymbol{\nu}_{t,s}$$



Background

Implementation and an alternative definition

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



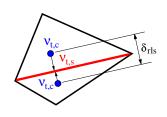
We can also compute an equivalent filter length,  $\tilde{\delta}_{\mathrm{rls}}$ , that leads to the same local dissipation

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

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

Implementation and an alternative definition

$${\color{red} \boldsymbol{\nu}_{t,c}} \xrightarrow{1/\delta_{vol}^2} \boldsymbol{\hat{\nu}}_{t,c} \xrightarrow{\text{interpolation}} \boldsymbol{\hat{\nu}}_{t,s} \xrightarrow{-\stackrel{\delta_{rls}^2}{-rls}} {\color{red} \boldsymbol{\nu}_{t,s}}$$



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

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

$$\boxed{ \tilde{\delta}_{\mathrm{rls}} = \sqrt{\frac{\hat{\mathsf{G}} : \hat{\mathsf{G}}}{\mathsf{G} : \mathsf{G}}} = \sqrt{\frac{\mathrm{tr}(\hat{\mathsf{G}}\hat{\mathsf{G}}^{\mathcal{T}})}{\mathrm{tr}(\mathsf{G}\mathsf{G}^{\mathcal{T}})}} }$$

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

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

$$\Delta = \left(\begin{array}{cc} \Delta x & 0 \\ 0 & \Delta y \end{array}\right)$$

$$\mathsf{G} = \left( \begin{array}{cc} \partial_x u & \partial_y u \\ \partial_y u & \partial_y v \end{array} \right)$$

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

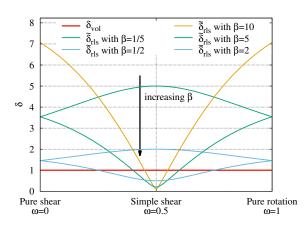
Background

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

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

Background

$$\Delta = \left( \begin{array}{cc} \Delta x & 0 \\ 0 & \Delta y \end{array} \right) = \left( \begin{array}{cc} \beta & 0 \\ 0 & \beta^{-1} \end{array} \right) \qquad \mathsf{G} = \left( \begin{array}{cc} \partial_x u & \partial_y u \\ \partial_y u & \partial_y v \end{array} \right) = \left( \begin{array}{cc} 0 & 1 \\ 1 - 2\omega & 0 \end{array} \right)$$

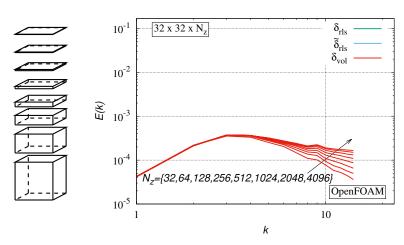


Isotropic turbulence on anisotropic grids

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

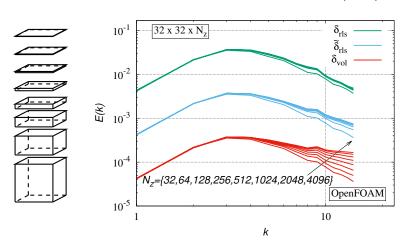
A rational length scale for LES

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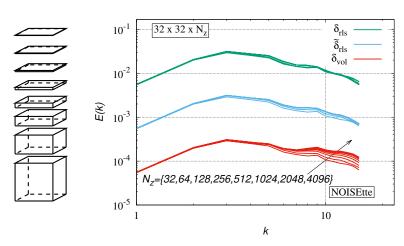
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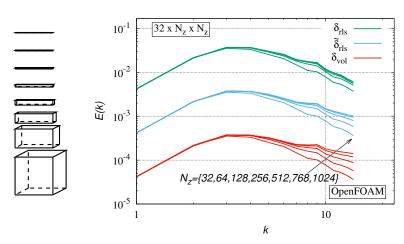


Isotropic turbulence on anisotropic grids

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

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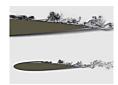
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#### Contents

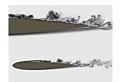
- Conclusions

 Preserving operator symmetries is the key point for reliable LES/DNS simulations



Background

- Preserving operator symmetries is the key point for reliable LES/DNS simulations
- Numerical schemes in FVM can be viewed as spatial (box) filters



$$\frac{\partial \varphi}{\partial t} + \frac{\partial (\mathbf{u}\varphi)}{\partial x} = \nu \frac{\partial^2 \varphi}{\partial x^2}$$

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

Background

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- Numerical schemes in FVM can be viewed as spatial (box) filters



$$\frac{\partial \varphi}{\partial t} + \frac{\partial (\mathbf{u}\varphi)}{\partial x} = \nu \frac{\partial^2 \varphi}{\partial x^2} \quad \stackrel{\text{schemes}}{\longrightarrow} \quad \left| \frac{\partial \varphi}{\partial t} + \frac{\overline{\partial (\mathbf{u}\overline{\varphi})}}{\partial x} \right| = \nu \frac{\overline{\partial^2 \overline{\varphi}}}{\partial x^2}$$

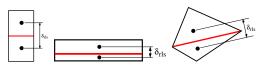
$$\boxed{\frac{\partial \varphi}{\partial t} + \overline{\frac{\partial (\mathbf{u}\overline{\varphi})}{\partial x}} = \nu \overline{\frac{\partial^2 \overline{\varphi}}{\partial x^2}}}$$

 In principle, the analysis can be extended to 3D problems and unstructured grids

$$\overline{\nabla^2 \varphi = \overline{\nabla^2 \overline{\varphi}} + \overline{\nabla^2 \varphi'} + (\nabla^2 \overline{\varphi})' + \mathcal{O}(h^4)}$$

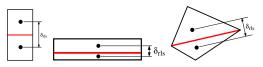


ullet A new definition for  $\delta$  has been proposed



$$ilde{\delta}_{
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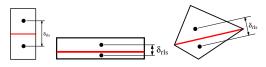


$$ilde{\delta}_{
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- It is locally defined, well-bounded, cheap and easy to implement
- Suitable for unstructured grids

Background

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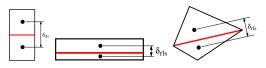


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- LES tests:
  - HIT
  - Turbulent channel flow (on-going)
  - Unstructured grids (future work)

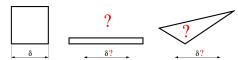
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Takeaway message:

ullet Definition of  $\delta$  can have a big effect on simulation results