

**Syver Døving Agdestein**

**CWI**

KWG afternoon session, Friday May 8, 2026

# **Data-driven discrete closure models**

*for large-eddy simulation of incompressible turbulence*

Large-eddy  
simulation

S. D. Agdestein

Simulating  
turbulence

Turbulence: an ancient  
problem

Simulation of turbulence

Large-eddy simulation

Issues with current closure  
models

Discrete LES

Symmetry-groups

Conclusion

250 BC



## Large-eddy simulation

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1500 AD



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1500 AD



2000 AD



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# Simulation of turbulence

## The incompressible Navier-Stokes equations

### Conservation of mass

$$\nabla \cdot u = 0$$

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### Conservation of momentum

$$\partial_t u + \nabla \cdot (uu - \nu \nabla u + p\delta) = f$$

## Conservation of mass

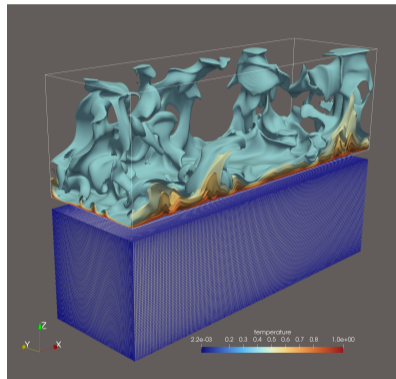
$$\nabla \cdot u = 0$$

## Conservation of momentum

$$\partial_t u + \nabla \cdot (uu - \nu \nabla u + p\delta) = f$$

# Simulation of turbulence

## The incompressible Navier-Stokes equations



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Filter out length scales smaller than  $\Delta$

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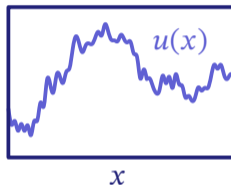
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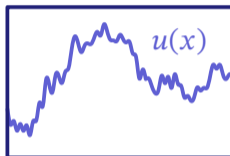
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## Turbulence

 $x$ 

$$L(u) = 0$$

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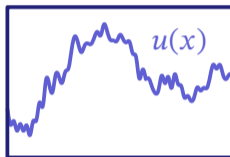
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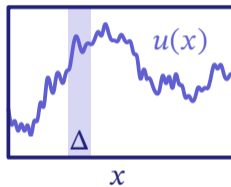
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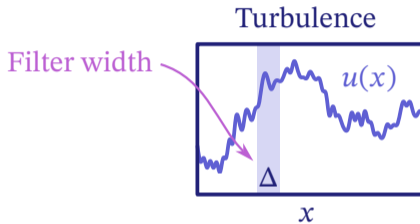
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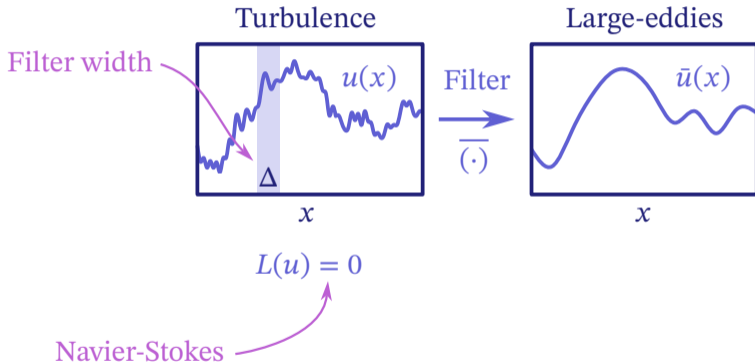
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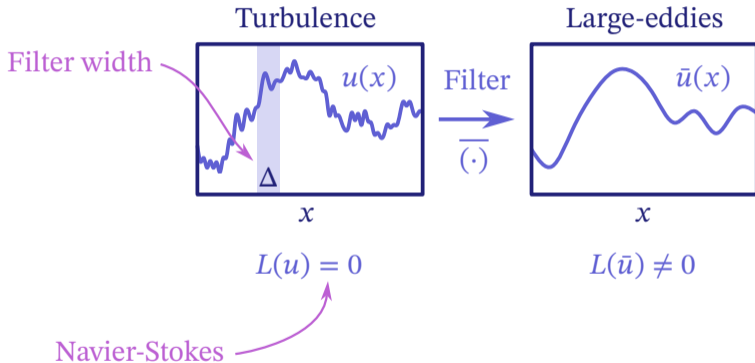
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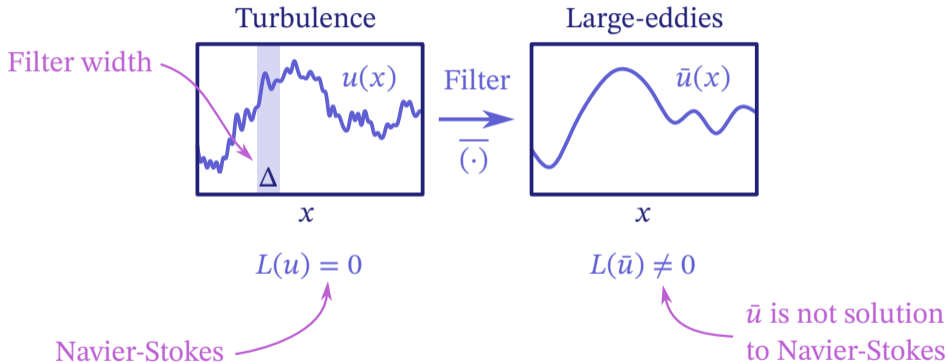
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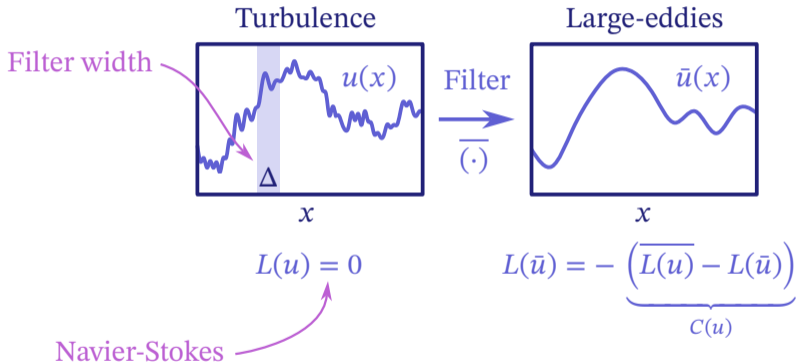
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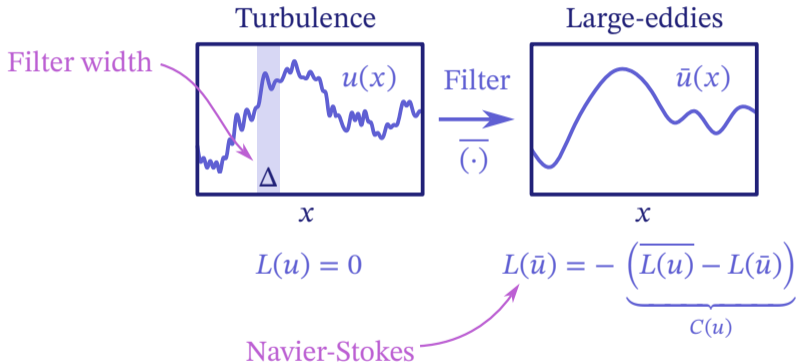
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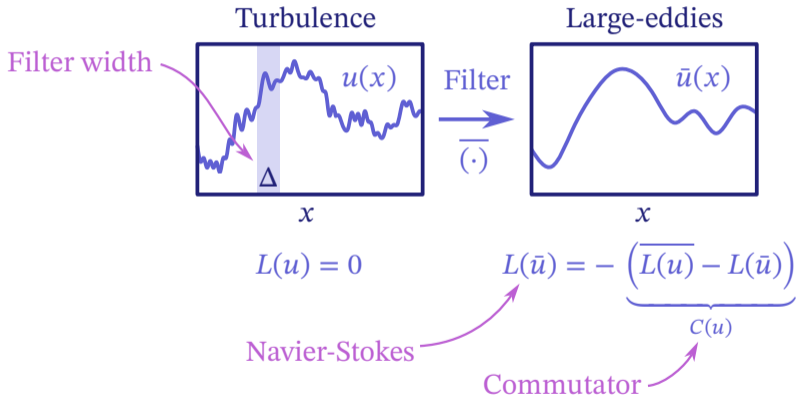
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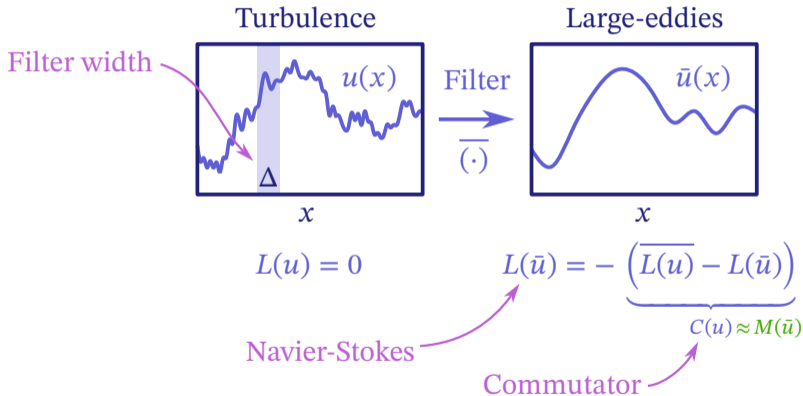
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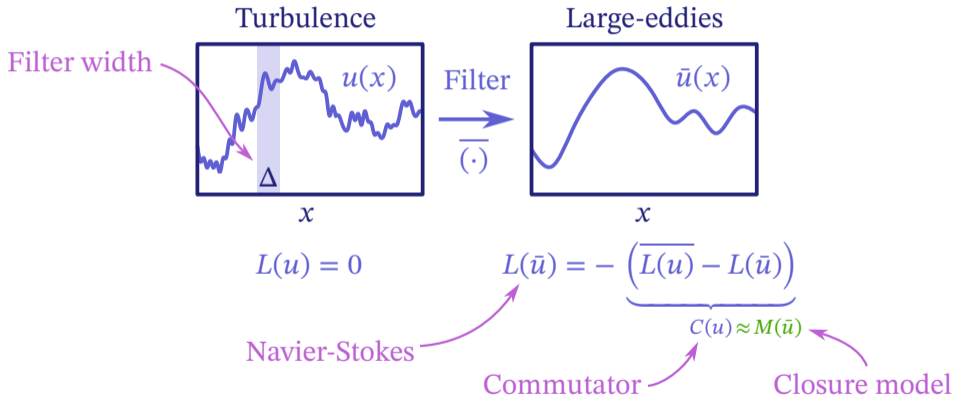
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**Issues with current closure models**

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# Issues with current closure models

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- Closure model  $M_\theta$  depends on parameters  $\theta$

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- Learn  $\theta$  from high-fidelity data  $\mathcal{D}$ :

$$\min_{\theta} \mathbb{E}_{u \sim \mathcal{D}} \|M_\theta(\bar{u}) - C(u)\|^2$$

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*There are other commutators than  $C(u)$ .  
They cause the instabilities.*

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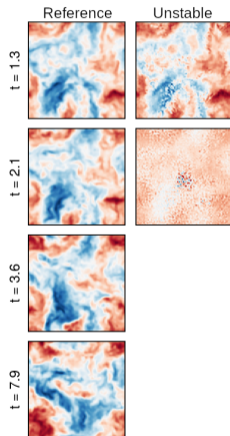
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## Identify all commutators

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## Identify all commutators

› from the filter  $\overline{(\cdot)}$

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**Identify all commutators**

- › from the filter  $\overline{(\cdot)}$
- › from the discretization  $\nabla_h$

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**Identify all commutators**

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**Address all commutators**

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- › Eliminate them by choosing  $\overline{(\cdot)}$ ,  $\nabla_h$ , and  $M_\theta$  in a smart way

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- › Eliminate them by choosing  $\overline{(\cdot)}$ ,  $\nabla_h$ , and  $M_\theta$  in a smart way
- › Account for the remaining ones by tuning the parameters  $\theta$

## Large-eddy simulation

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Discretize first

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# A new framework: discretize first

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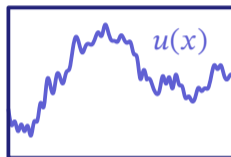
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$x$

$$L(u) = 0$$

Navier-Stokes



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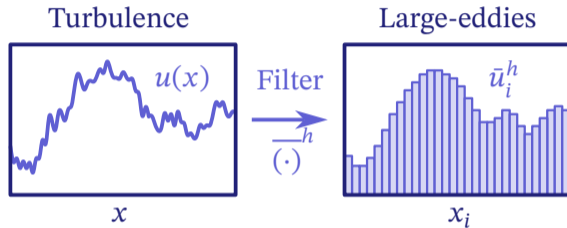
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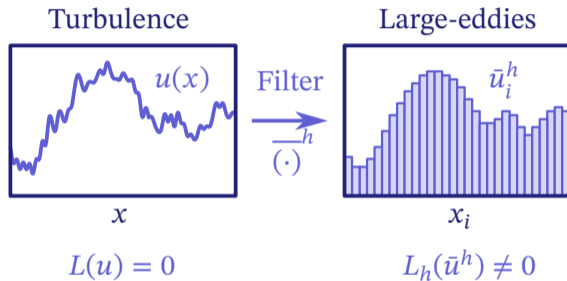
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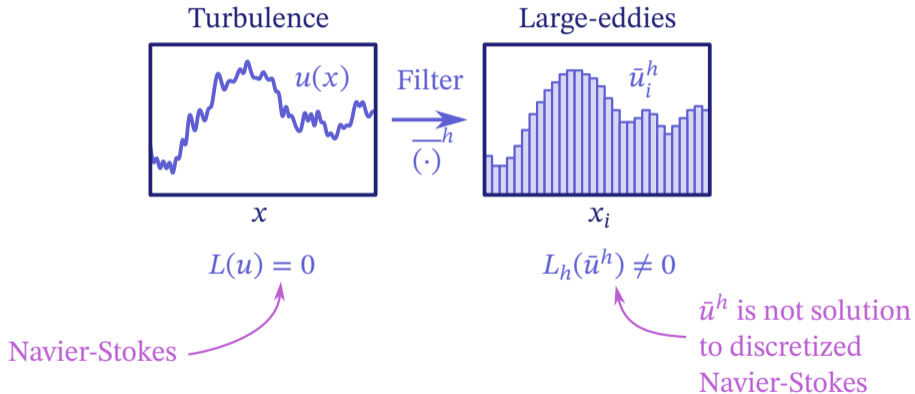
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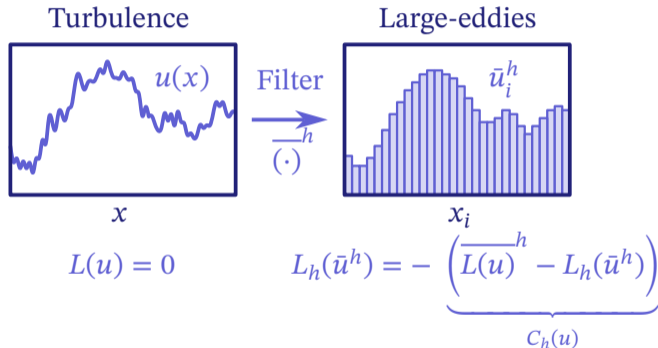
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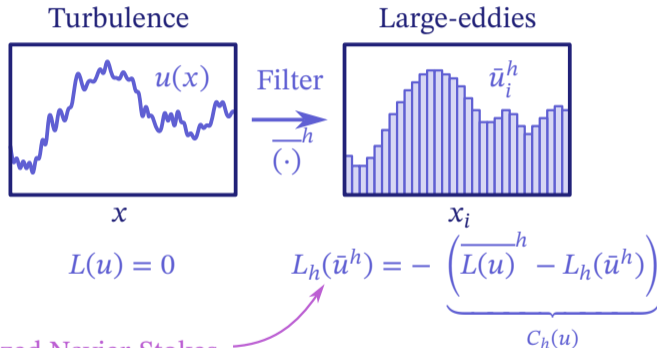
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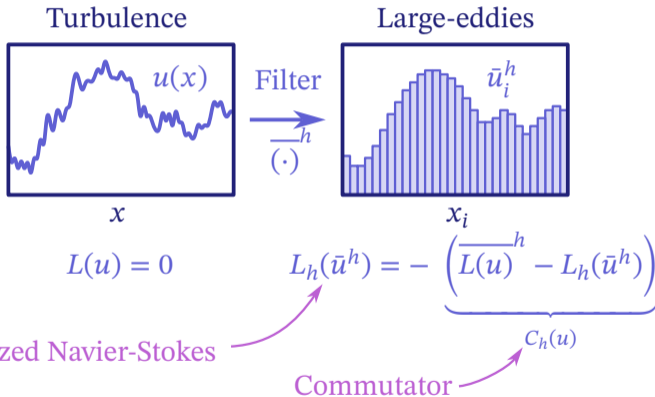
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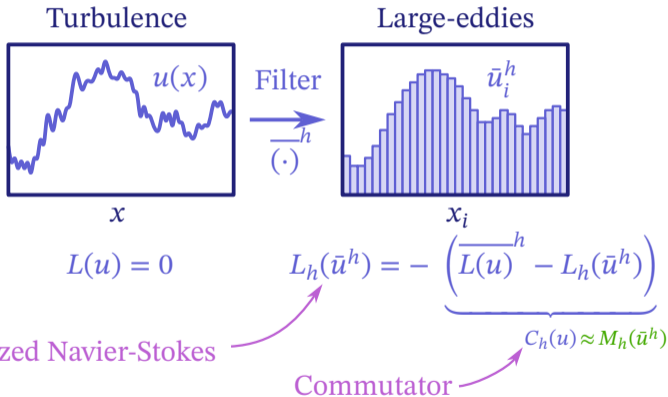
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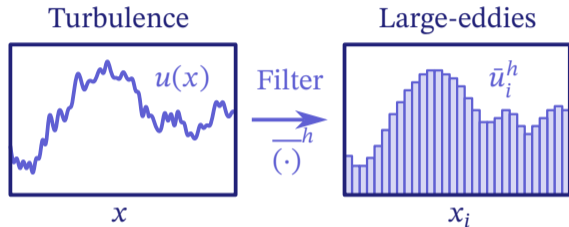
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$$L(u) = 0$$

$$L_h(\bar{u}^h) = - \underbrace{\left( \overline{L(u)}^h - L_h(\bar{u}^h) \right)}$$

Discretized Navier-Stokes

Commutator

$$C_h(u) \approx M_h(\bar{u}^h)$$

Closure model

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# New filters, new stresses

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## Discrete filters

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## Discrete filters

- Existing discrete filters induce discrete commutator errors.

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## Discrete filters

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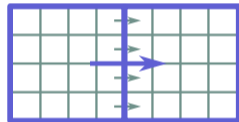
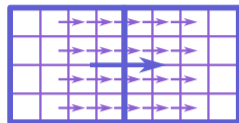
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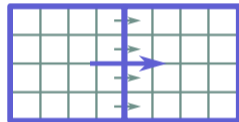
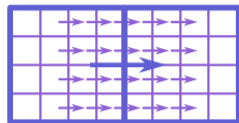


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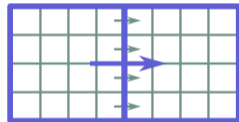
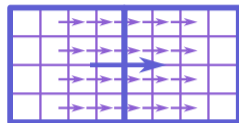
## Stress tensors in LES

## New filters, new stresses



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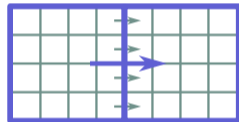
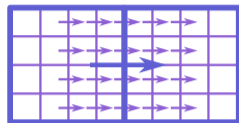


## Stress tensors in LES

- Continuous LES stress expressions are symmetric and local in  $u$ .

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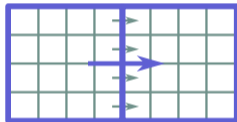
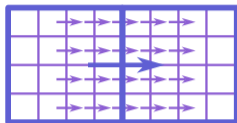


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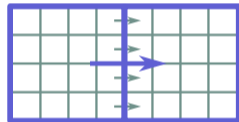
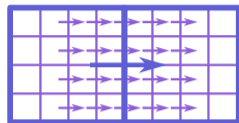
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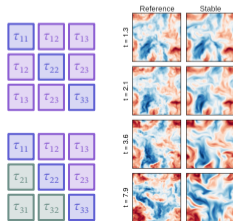
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# Symmetries of the Navier-Stokes equations

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# Symmetries of the Navier-Stokes equations

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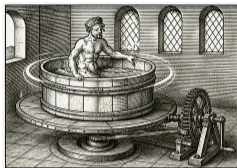
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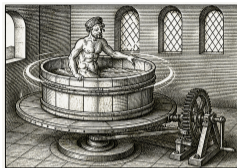
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*$G$  is a symmetry-group of the Navier-Stokes equations  $L$  if and only if*

$$L(gu) = gL(u)$$

*for all velocities  $u$  and group elements  $g \in G$ .*

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*How to choose  $M_\theta$  such that  $M_\theta(g\bar{u}) = gM_\theta(\bar{u})$  for all  $\theta$ ,  $\bar{u}$ , and  $g \in G$ ?*

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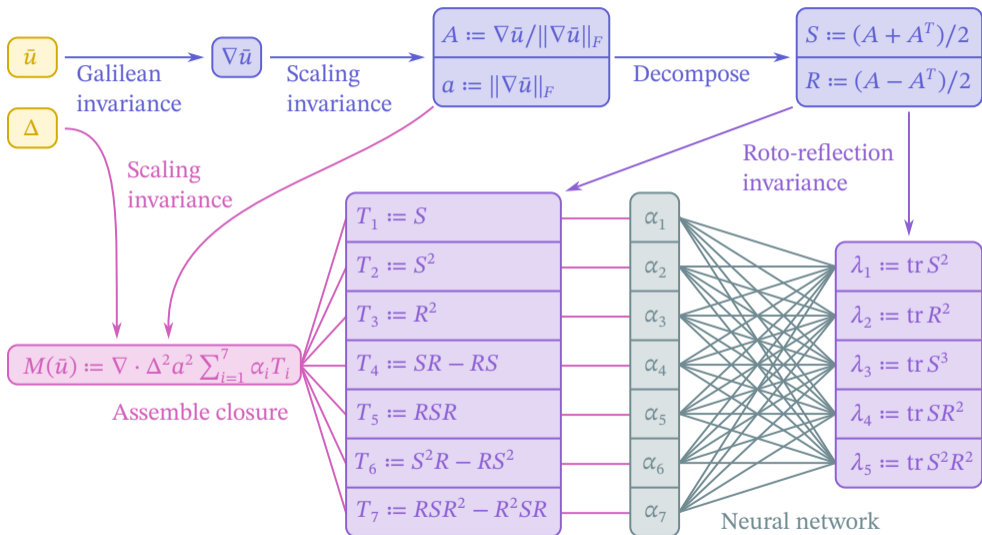
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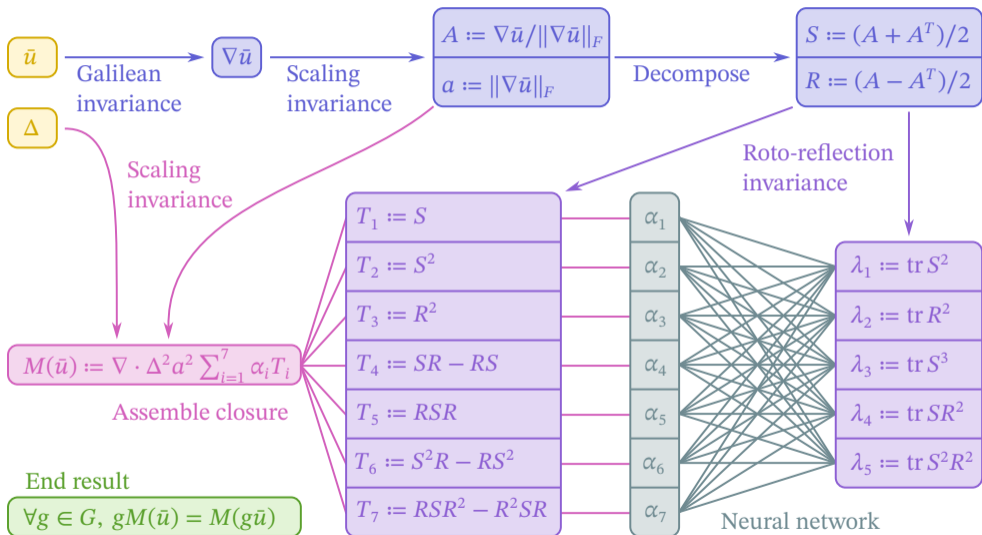
# Tensor basis neural network

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# Tensor basis neural network



# Tensor basis neural network



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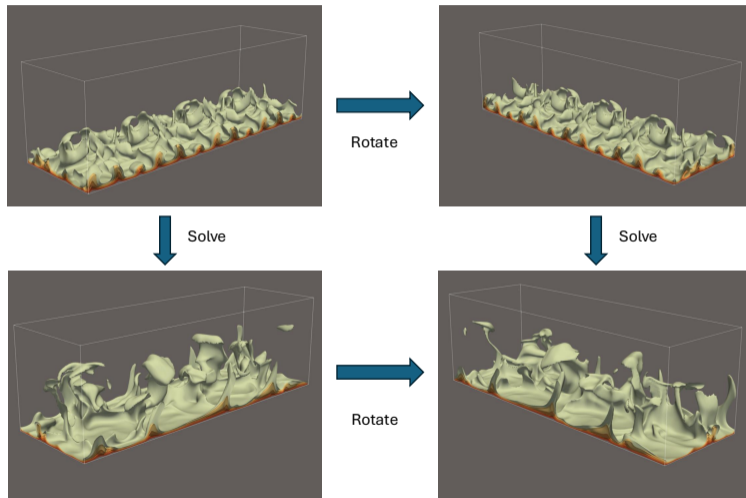
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Thank you!

# Take-away

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*The main problem in LES is the presence of commutator errors.*

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Thank you!

*The main problem in LES is the presence of commutator errors.*

*We identify new commutators in LES arising from the filter, discretization, and symmetry-groups.*

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Thank you!

*The main problem in LES is the presence of commutator errors.*

*We identify new commutators in LES arising from the filter, discretization, and symmetry-groups.*

*We cancel out commutators through new filters, discrete formulations, and model architectures.*

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Thank you!

*The main problem in LES is the presence of commutator errors.*

*We identify new commutators in LES arising from the filter, discretization, and symmetry-groups.*

*We cancel out commutators through new filters, discrete formulations, and model architectures.*

*Exact expressions for the remaining commutators allow for producing unbiased training data for data-driven closure models.*

*The main problem in LES is the presence of commutator errors.*

*We identify new commutators in LES arising from the filter, discretization, and symmetry-groups.*

*We cancel out commutators through new filters, discrete formulations, and model architectures.*

*Exact expressions for the remaining commutators allow for producing unbiased training data for data-driven closure models.*

*This thesis offers a mathematically principled foundation for reducing the computational cost of turbulence simulations.*

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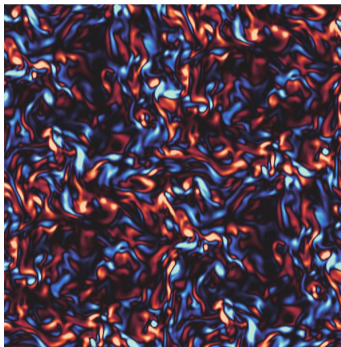
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# Thank you!



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# Lifecycle of turbulence

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## The Burgers' equation (1D)

$$\partial_t u = \underbrace{\nu \partial_{xx} u}_{\text{Diffusion}} - \underbrace{\partial_x (u^2/2)}_{\text{Convection}}$$

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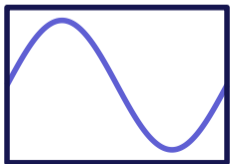
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## The Burgers' equation (1D)

$$\partial_t u = \underbrace{\nu \partial_{xx} u}_{\text{Diffusion}} - \underbrace{\partial_x (u^2/2)}_{\text{Convection}}$$

## Effect on a Fourier mode

$$u = e^{ikx}$$

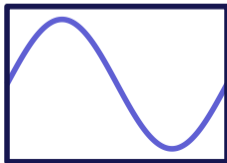


## The Burgers' equation (1D)

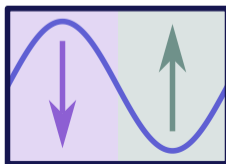
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$$u = e^{ikx}$$



$$\partial_{xx} u = -k^2 e^{ikx}$$

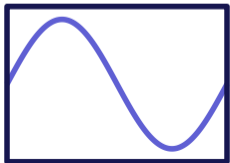


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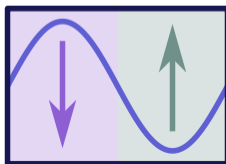
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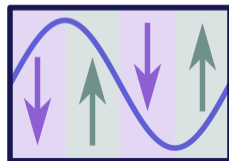
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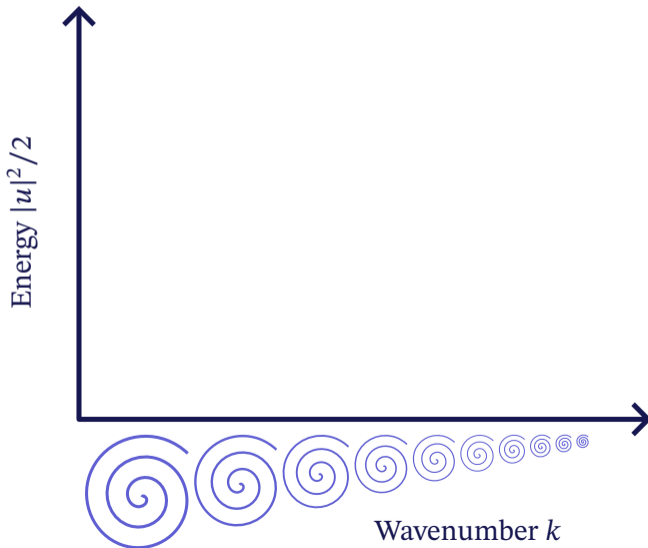
$$\partial_x (u^2/2) = ike^{i(2k)x}$$



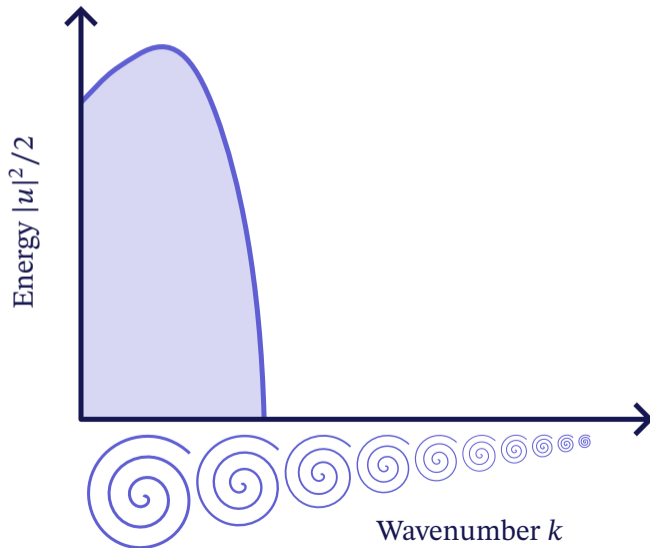
# Spectral distribution of energy

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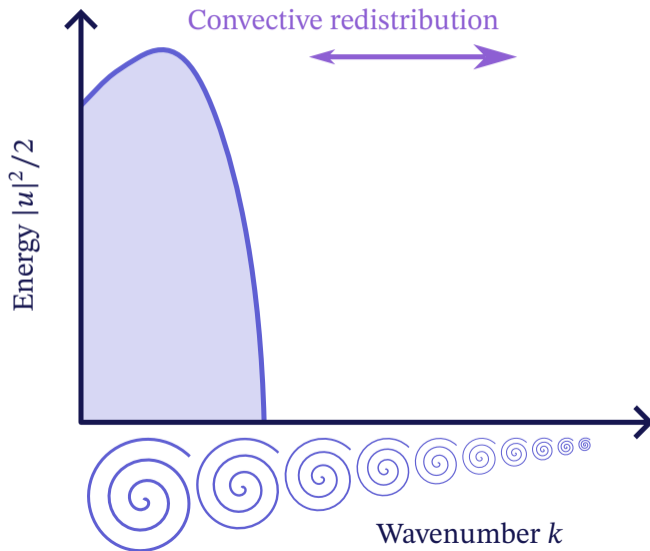
# Spectral distribution of energy



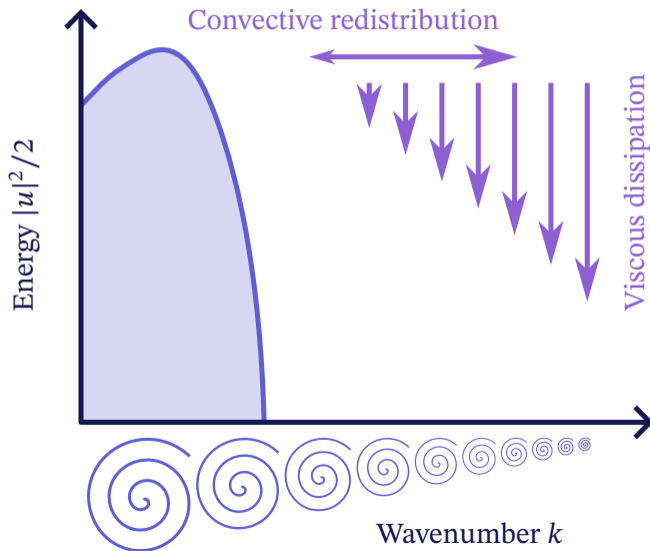
# Spectral distribution of energy



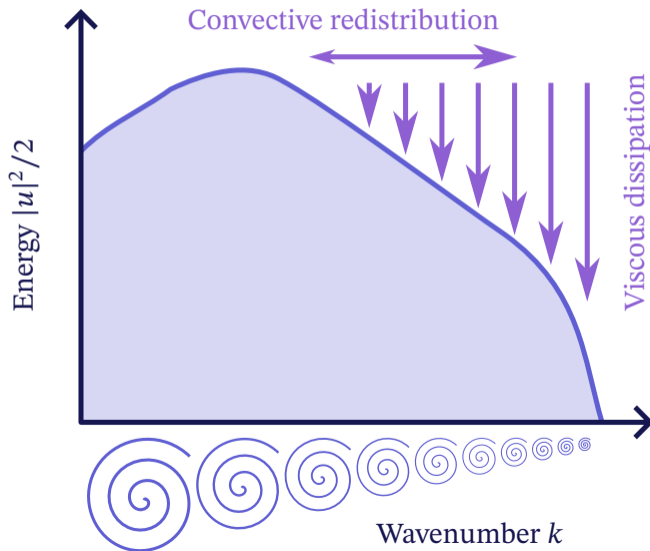
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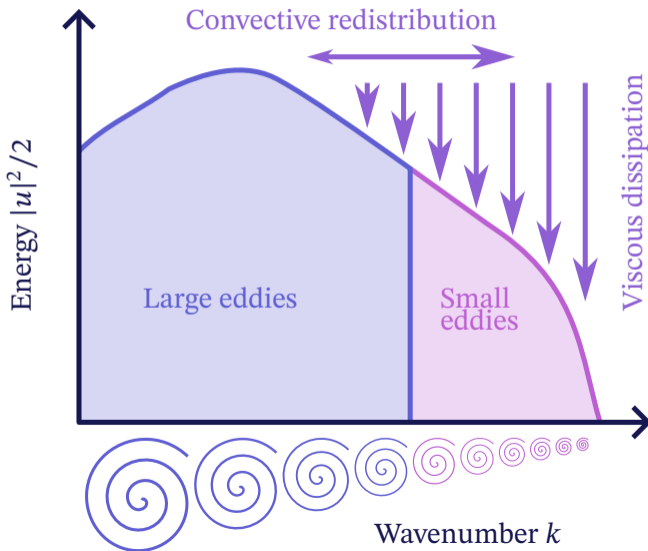
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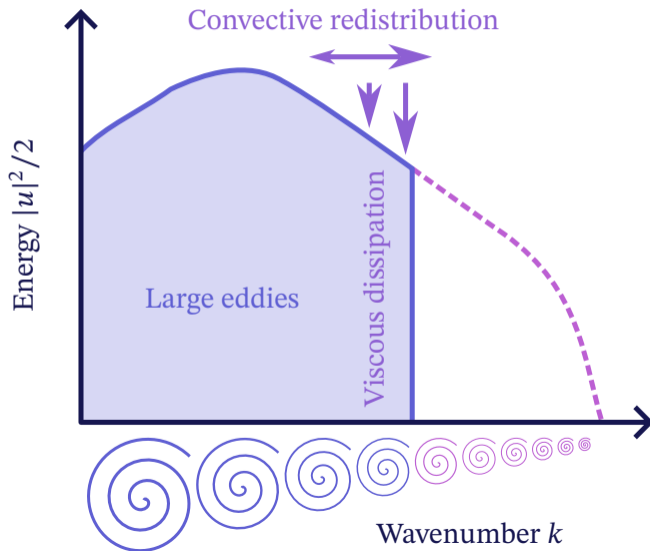
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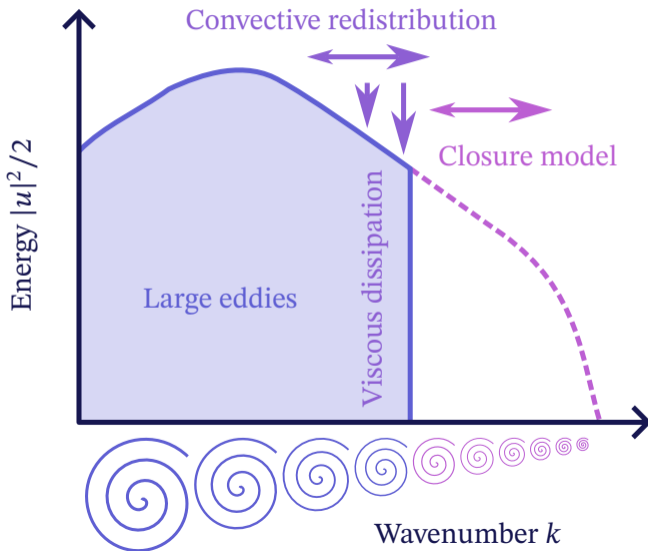
# Spectral distribution of energy



# Spectral distribution of energy



# Spectral distribution of energy



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# Issues with state of the art

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Closure model target:

$$C(u) = \nabla \cdot \underbrace{[\overline{uu} - \bar{u}\bar{u}]}_{-\frac{\Delta^2}{12} \nabla \bar{u} \nabla \bar{u}^T + \mathcal{O}(\Delta^4)}$$

Closure model target:

$$C(u) = \nabla \cdot \underbrace{[\overline{uu} - \bar{u}\bar{u}]}_{-\frac{\Delta^2}{12} \nabla \bar{u} \nabla \bar{u}^T + \mathcal{O}(\Delta^4)}$$

---

## Structural models: Unstable

$$M(\bar{u}) = \nabla \cdot \left[ -\frac{\Delta^2}{12} \nabla \bar{u} \nabla \bar{u}^T \right]$$

Closure model target:

$$C(\mathbf{u}) = \nabla \cdot \underbrace{[\overline{\mathbf{u}\mathbf{u}} - \bar{\mathbf{u}}\bar{\mathbf{u}}]}_{-\frac{\Delta^2}{12}\nabla\bar{\mathbf{u}}\nabla\bar{\mathbf{u}}^T + \mathcal{O}(\Delta^4)}$$

**Structural models: Unstable**

$$M(\bar{\mathbf{u}}) = \nabla \cdot \left[ -\frac{\Delta^2}{12} \nabla\bar{\mathbf{u}}\nabla\bar{\mathbf{u}}^T \right]$$

**Functional models: Inaccurate**

$$M(\bar{\mathbf{u}}) = \nabla \cdot \left[ -\nu_{\text{eddy}} (\nabla\bar{\mathbf{u}} + \nabla\bar{\mathbf{u}}^T) \right]$$

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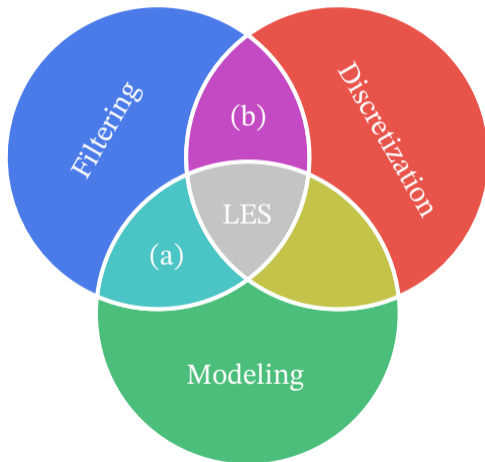
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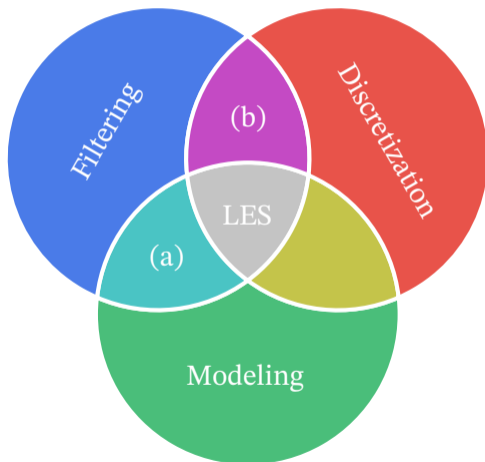
# Discretization-aware LES

Correcting for an inconsistency in the data



# Discretization-aware LES

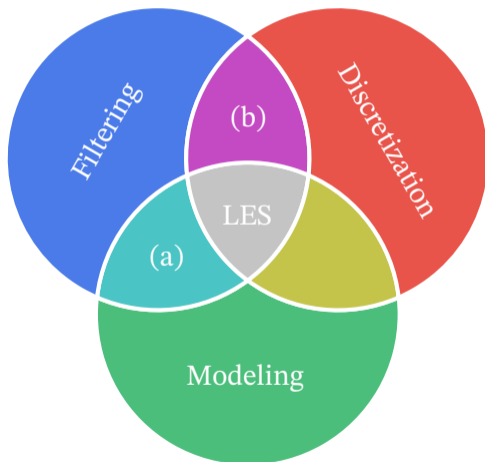
Correcting for an inconsistency in the data



# Discretization-aware LES

Correcting for an inconsistency in the data

- a** Classical approach: Filter and model, then discretize



# Discretization-aware LES

Correcting for an inconsistency in the data

- a** Classical approach: Filter and model, then discretize
- b** New approach: Filter and discretize, then model

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# Exact discrete stress

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## With pressure and constraint

$$\nabla \cdot \mathbf{u} = 0, \quad \partial_t \mathbf{u} = -\nabla \cdot (\boldsymbol{\sigma}(\mathbf{u}) + p\boldsymbol{\delta})$$

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## With pressure and constraint

$$\nabla \cdot \mathbf{u} = 0, \quad \partial_t \mathbf{u} = -\nabla \cdot (\boldsymbol{\sigma}(\mathbf{u}) + p\boldsymbol{\delta})$$

## Pressure-free formulation

$$\partial_t \mathbf{u} = -\nabla \cdot \boldsymbol{\pi} \boldsymbol{\sigma}(\mathbf{u}), \quad \pi_{ij\alpha\beta} := \delta_{i\alpha} \delta_{j\beta} - \delta_{ij} (\partial_k \partial_k)^\dagger \partial_\alpha \partial_\beta$$

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## With pressure and constraint

$$\nabla \cdot \mathbf{u} = 0, \quad \partial_t \mathbf{u} = -\nabla \cdot (\boldsymbol{\sigma}(\mathbf{u}) + p\boldsymbol{\delta})$$

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## Exact LES equations

$$\text{Infinitesimal LES: } \partial_t \bar{\mathbf{u}} = -\overline{\nabla \cdot \boldsymbol{\pi} \boldsymbol{\sigma}(\mathbf{u})} = -\nabla \cdot \overline{\boldsymbol{\pi} \boldsymbol{\sigma}(\mathbf{u})}$$

$$\text{Discrete LES: } \partial_t \bar{\mathbf{u}}^h = -\overline{\nabla \cdot \boldsymbol{\pi} \boldsymbol{\sigma}(\mathbf{u})}^h = -\nabla_h \cdot \overline{\boldsymbol{\pi} \boldsymbol{\sigma}(\mathbf{u})}^{h,*}$$

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