Syver Døving Agdestein
syver.agdestein@cwi.nl
https://agdestein.github.io/

Centrum Wiskunde & Informatica

December 16, 2025

Data-driven closure modeling

From deterministic to probabilistic models

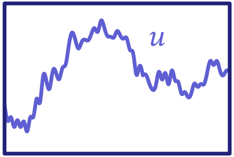
In collaboration with Benjamin Sanderse and Roel Verstappen

Closure modeling in large-eddy simulation

Large-eddy simulation (LES)

Filter and close

Turbulence

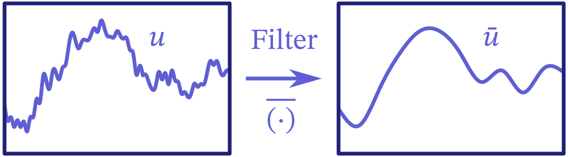


$$L(u) = 0$$

Large-eddy simulation (LES)

Filter and close

Turbulence | LES solution

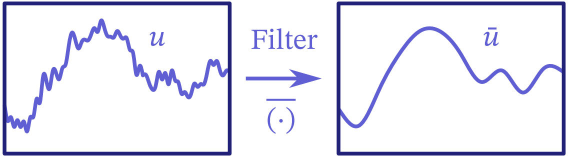


$L(u) = 0$ | $\overline{L(u)} = 0$

Large-eddy simulation (LES)

Filter and close

Turbulence | LES solution



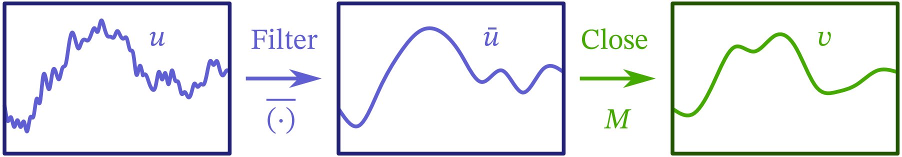
$$L(u) = 0$$

$$L(\bar{u}) = -\underbrace{\left(\overline{L(u)} - L(\bar{u})\right)}_{C(u)}$$

Large-eddy simulation (LES)

Filter and close

Turbulence | LES solution | LES approximation



$L(u) = 0$ | $L(\bar{u}) = -\underbrace{\left(\overline{L(u)} - L(\bar{u})\right)}_{C(u)}$ | $L(v) = -M(v)$

Data-driven closure

Training a neural network

Fitting model parameters θ to data $\mathcal{D}$:

$$\min_\theta \mathbb{E}_{u \sim \mathcal{D}} J_\theta(u)$$

The a-priori error

$$J_\theta(u) := \|M_\theta(\bar{u}) - C(u)\|^2.$$

The a-posteriori error

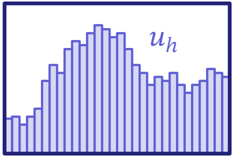
$$J_\theta(u) := \|v_\theta - \bar{u}\|^2, \quad v_\theta \text{ solution to } L(v) = -M_\theta(v).$$

Sanderse et al. 2025.

The discrete perspective

Consistent data from coarse-graining

Turbulence (DNS)

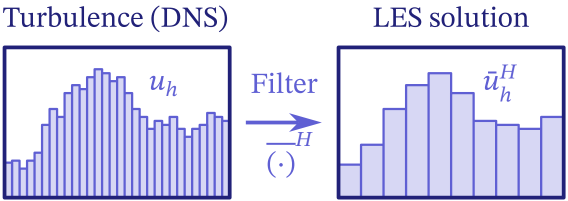


$$L_h(u_h) = 0$$

Agdestein and Sanderse 2025; Agdestein, Verstappen, and Sanderse 2025.

The discrete perspective

Consistent data from coarse-graining

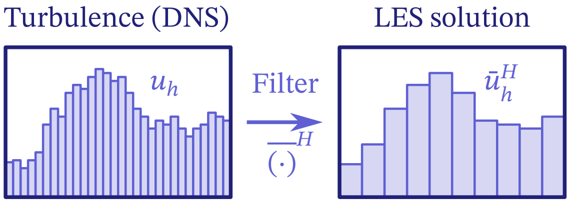


$$L_h(u_h) = 0 \qquad \overline{L_h(u_h)}^H = 0$$

Agdestein and Sanderse 2025; Agdestein, Verstappen, and Sanderse 2025.

The discrete perspective

Consistent data from coarse-graining



$$L_h(u_h) = 0$$

$$L_H(\bar{u}_h^H) = -C_H(u_h)$$

$$C_H(u_h) := \overline{L_h(u_h)}^H - L_H(\bar{u}_h^H)$$

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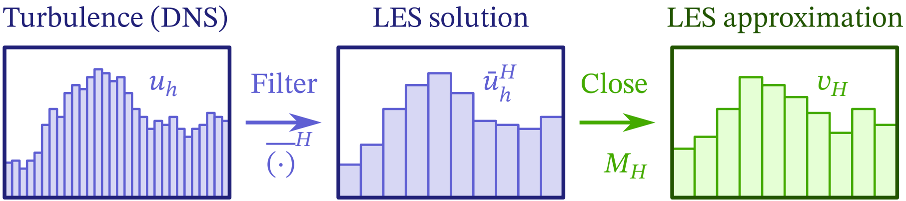
The discrete perspective

Consistent data from coarse-graining



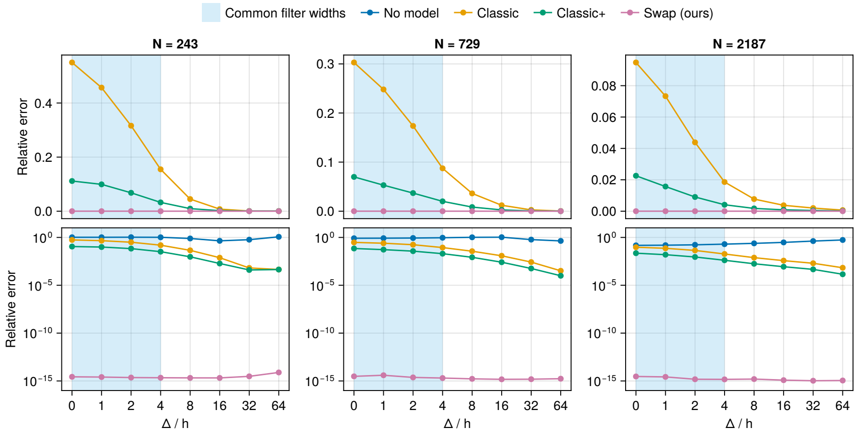
$$L_h(u_h) = 0 \qquad L_H(\bar{u}_h^H) = -C_H(u_h) \qquad L_H(v_H) = -M_H(v_H)$$

$$C_H(u_h) := \overline{L_h(u_h)}^H - L_H(\bar{u}_h^H)$$

Agdestein and Sanderse 2025; Agdestein, Verstappen, and Sanderse 2025.

The commutator expression is important

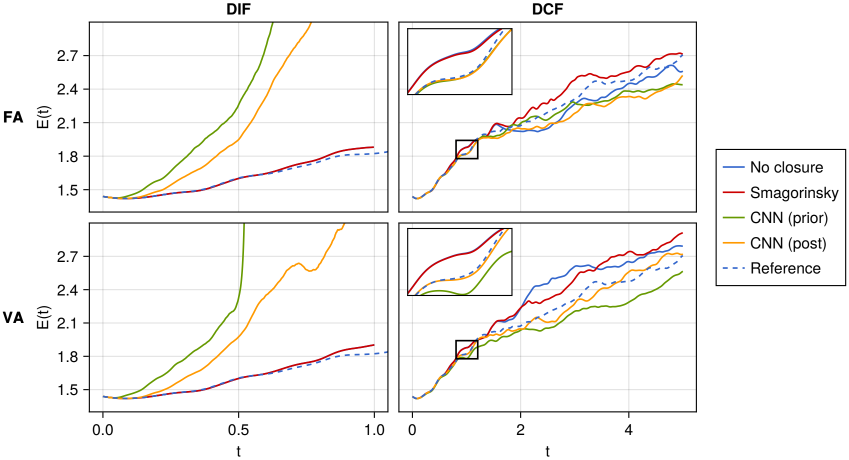
"DNS-aided LES" for Burgers' equation



Agdestein, Verstappen, and Sanderse 2025.

The commutator expression is important

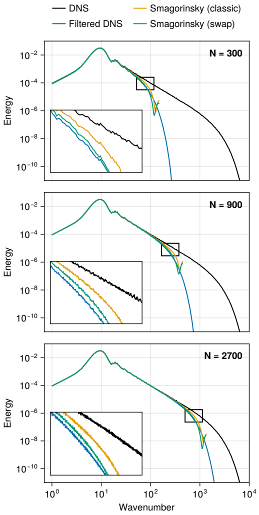
A-priori and a-posteriori learning



Agdestein and Sanderse 2025.

The commutator expression is important

Fitting a Smagorinsky model



$$S := (\nabla + \nabla^T)/2$$

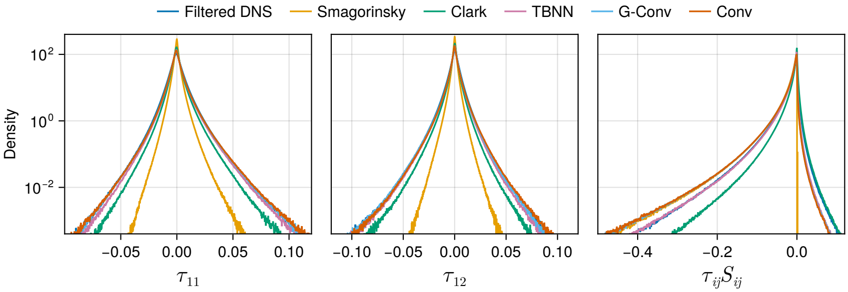
$$S_H := (\nabla_H + \nabla_H^T)/2$$

$$M(\bar{u}) := -\nabla \cdot 2\theta^2 \Delta^2 |S(\bar{u})| S(\bar{u})$$

$$M_H(\bar{u}_H) := -\nabla_H \cdot 2\theta^2 \Delta^2 |S_H(\bar{u}_H)| S_H(\bar{u}_H)$$

Incorporating symmetries

Tensor basis and group-convolutions



Cohen and Welling 2016; Ling, Kurzawski, and Templeton 2016.

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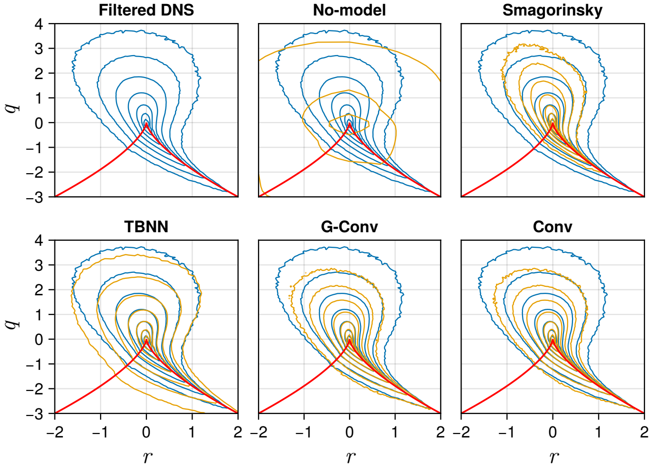


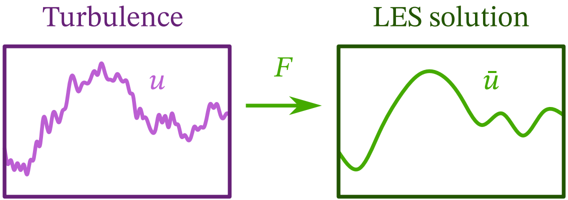
Cohen and Welling 2016; Ling, Kurzawski, and Templeton 2016.

Towards probabilistic closure models

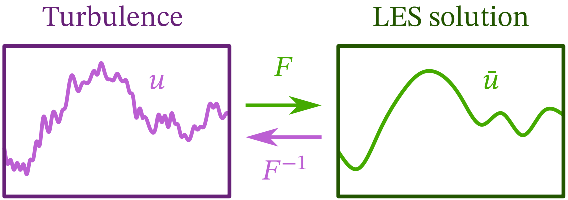
Motivation for probabilistic LES

Turbulence

Motivation for probabilistic LES



Motivation for probabilistic LES

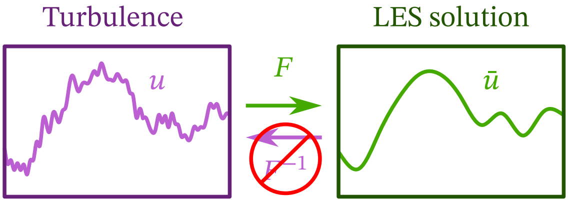


CWI

LES closure

S. D. Agdestein

Motivation for probabilistic LES



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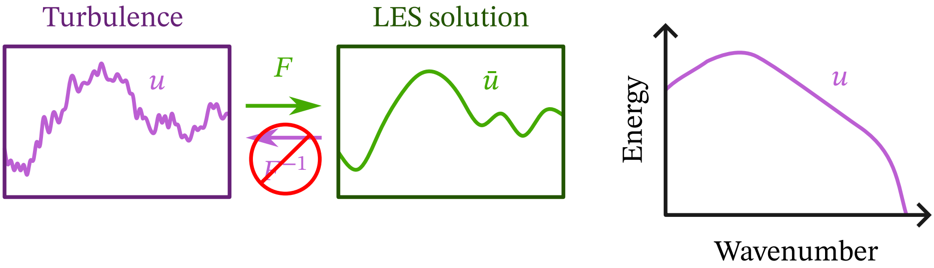

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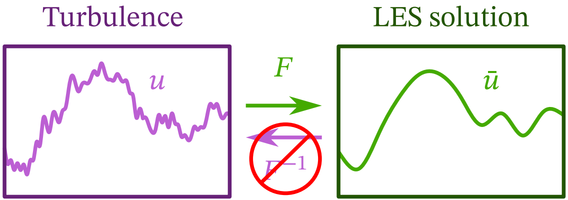

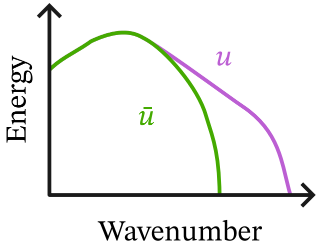

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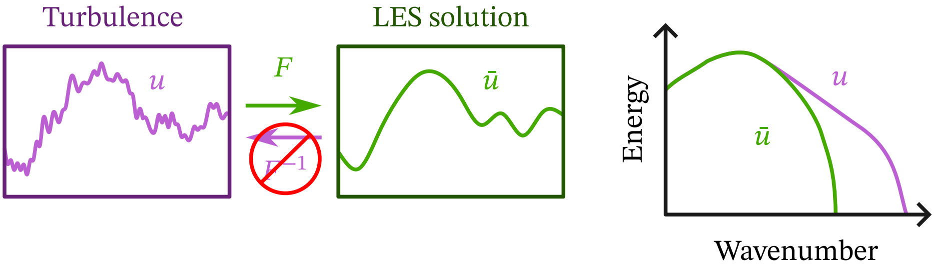

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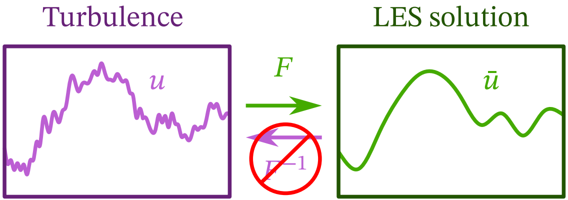

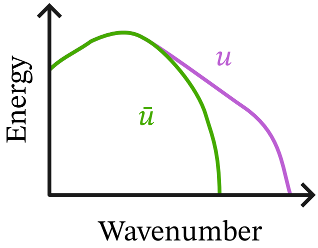

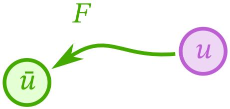

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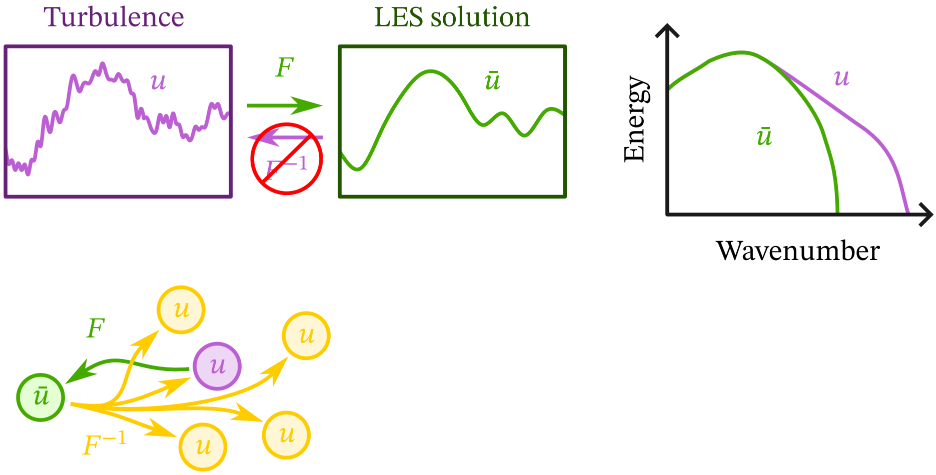

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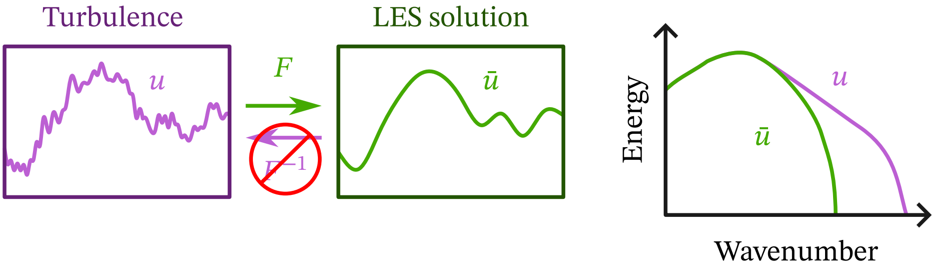
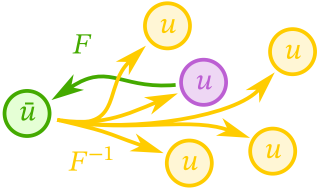
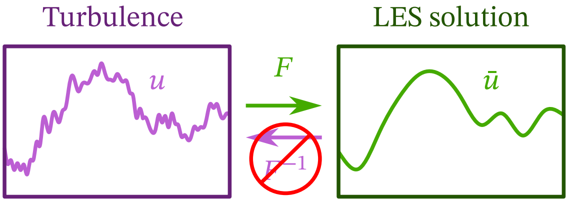
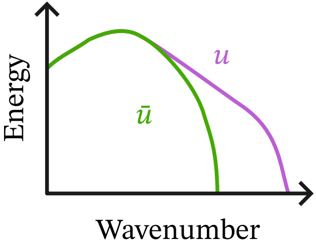


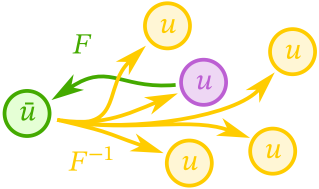


All these u's are equally likely
since they give the same $\bar{u}$.

Motivation for probabilistic LES







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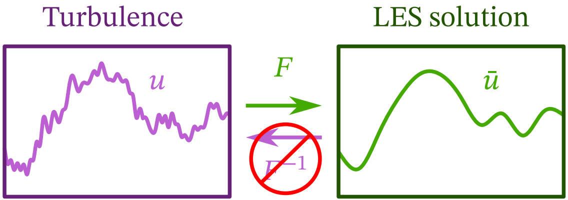
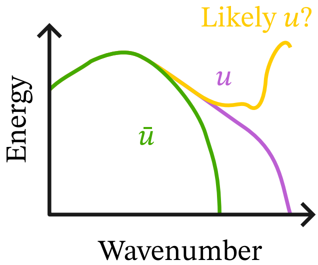
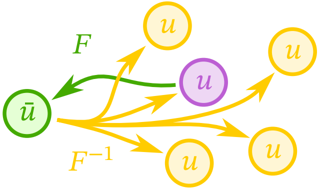
But some u's are more likely than others.

Motivation for probabilistic LES







All these u's are equally likely

since they give the same $\bar{u}$.

But some u's are more likely than others.

LES in the language of probability

The commutator distribution

Langford and Moser 1999; Pope 2004.

LES in the language of probability

The commutator distribution

$$p(u \mid \bar{u})$$

$$\uparrow F^{-1}$$

$$\bar{u}$$

Langford and Moser 1999; Pope 2004.

LES in the language of probability

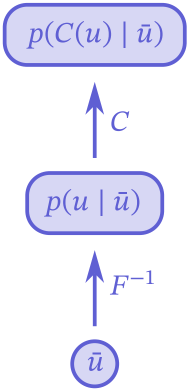
The commutator distribution

$$\bar{u} \xrightarrow{F^{-1}} p(u \mid \bar{u}) \xrightarrow{C} p(C(u) \mid \bar{u})$$

Langford and Moser 1999; Pope 2004.

LES in the language of probability

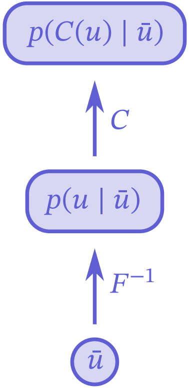
The commutator distribution

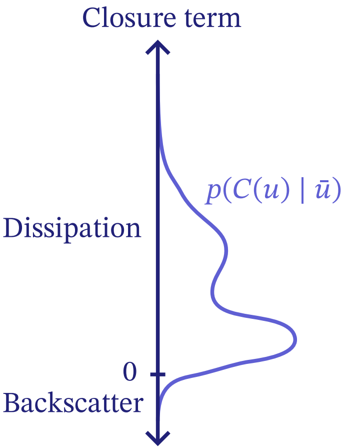


Langford and Moser 1999; Pope 2004.

LES in the language of probability

The commutator distribution





Langford and Moser 1999; Pope 2004.

LES in the language of probability

The commutator distribution

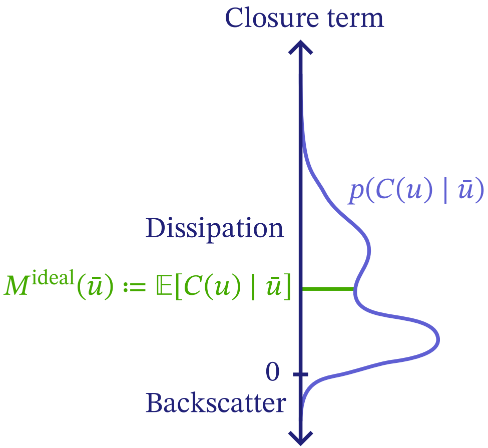
$$p(C(u) \mid \bar{u})$$

$$\uparrow C$$

$$p(u \mid \bar{u})$$

$$\uparrow F^{-1}$$

$$\bar{u}$$



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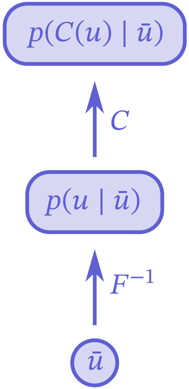
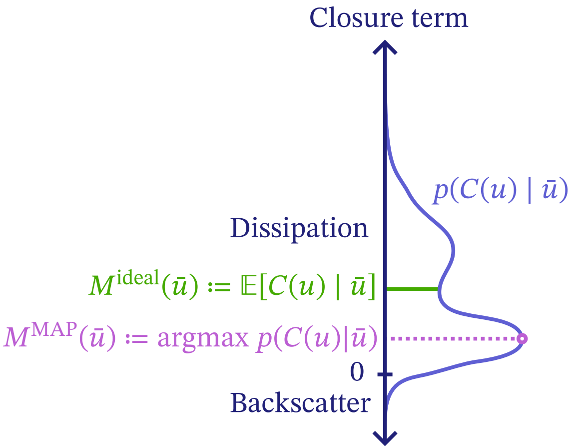
LES in the language of probability

The commutator distribution





Langford and Moser 1999; Pope 2004.

The Bayesian perspective

Balancing prior knowledge and data

Likelihood

Prior

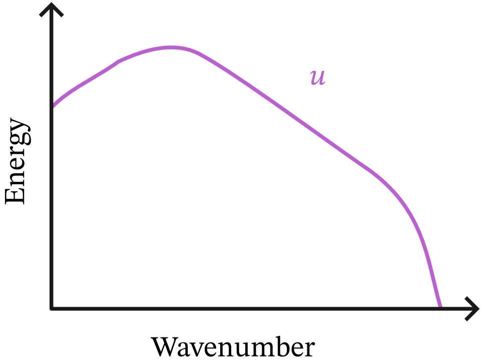
Posterior

$$\underbrace{p(u \mid \bar{u})}_{\text{Posterior}} = \frac{\overbrace{p(\bar{u} \mid u)}^{\text{Likelihood}} \, \overbrace{p(u)}^{\text{Prior}}}{\underbrace{p(\bar{u})}_{\text{Just some constant}}}$$

Just some constant

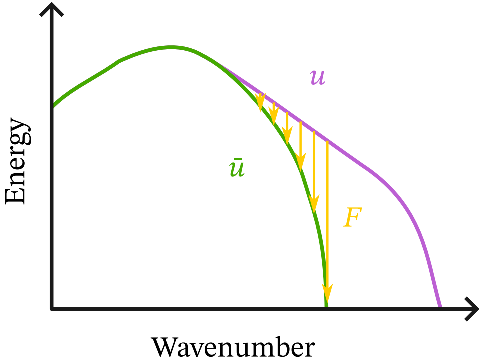
How do we sample?

Ad-hoc approaches



How do we sample?

Ad-hoc approaches



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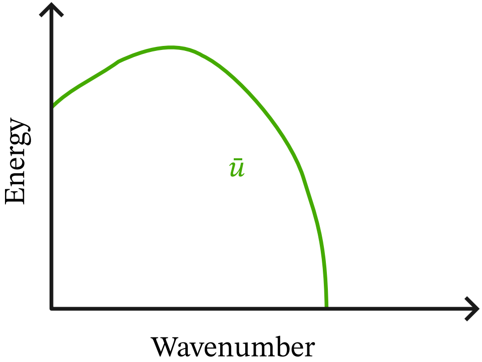

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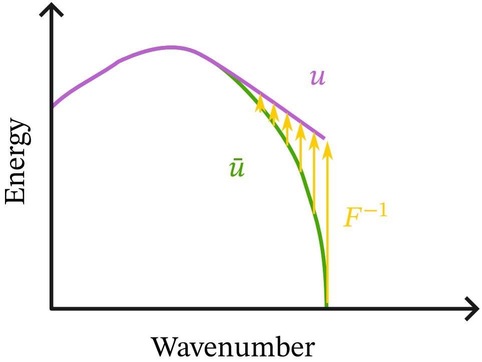
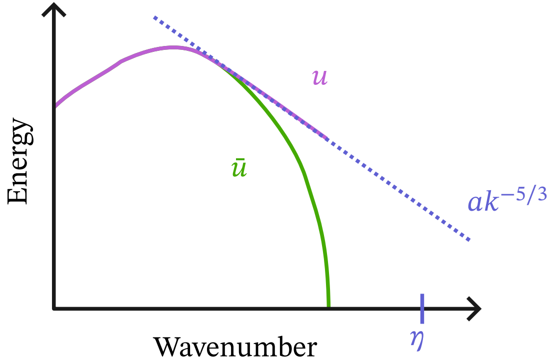


How do we sample?

Ad-hoc approaches



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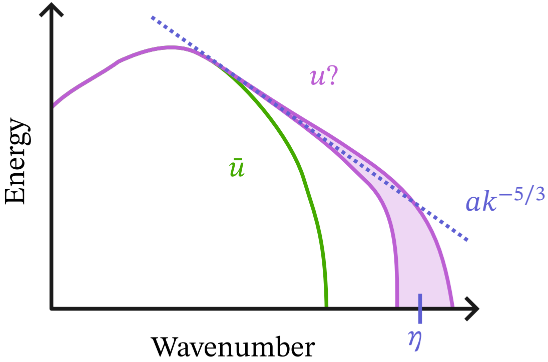
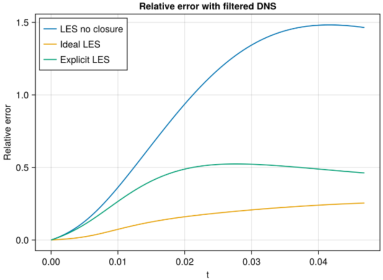
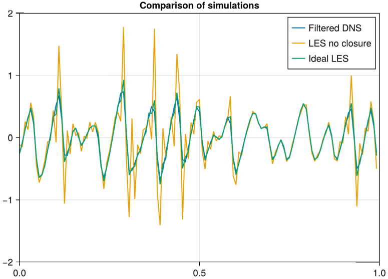
Ad-hoc approaches



Ad-hoc deconvolution

Spectral reconstruction in Burgers' equation

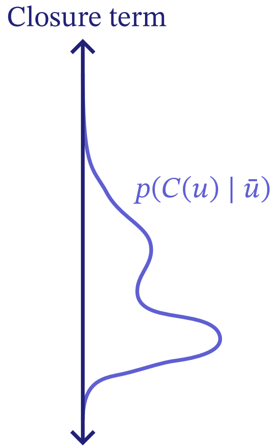




Lucas Ronckers, Master's thesis, 2025

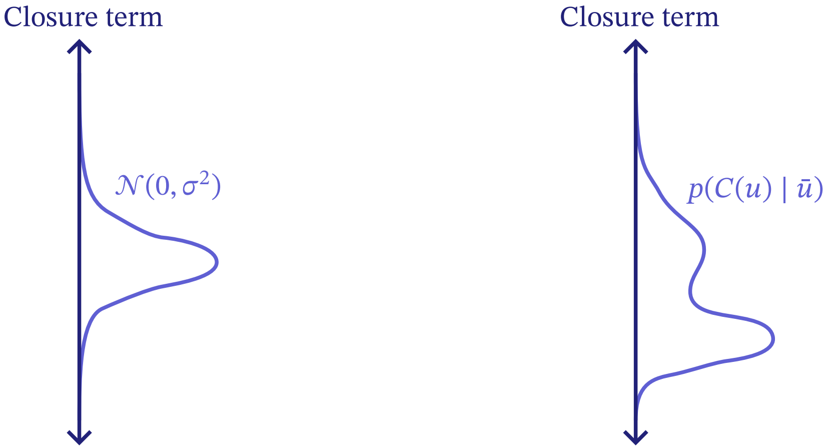
Data-driven sampling

Generative modeling



Data-driven sampling

Generative modeling



Data-driven sampling

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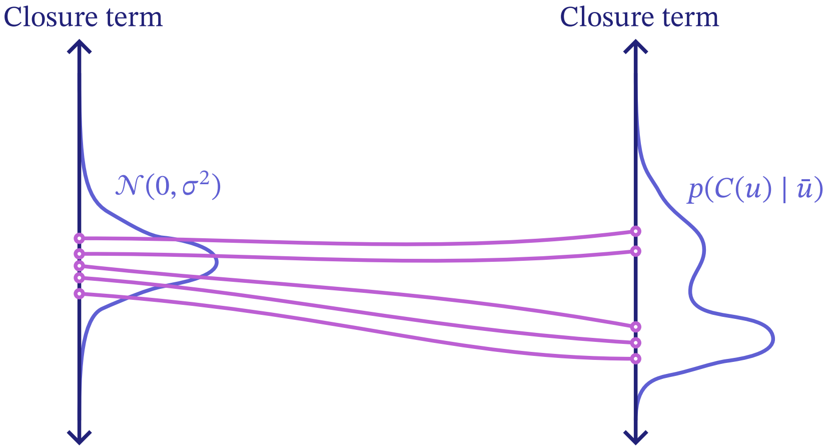

Data-driven sampling

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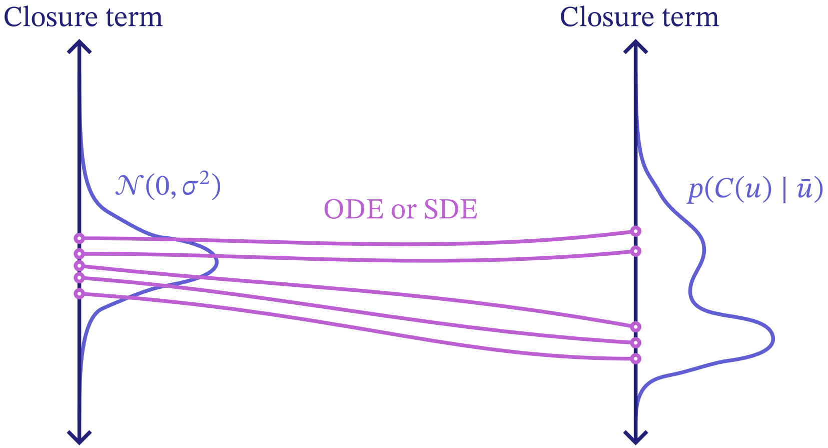

Data-driven sampling

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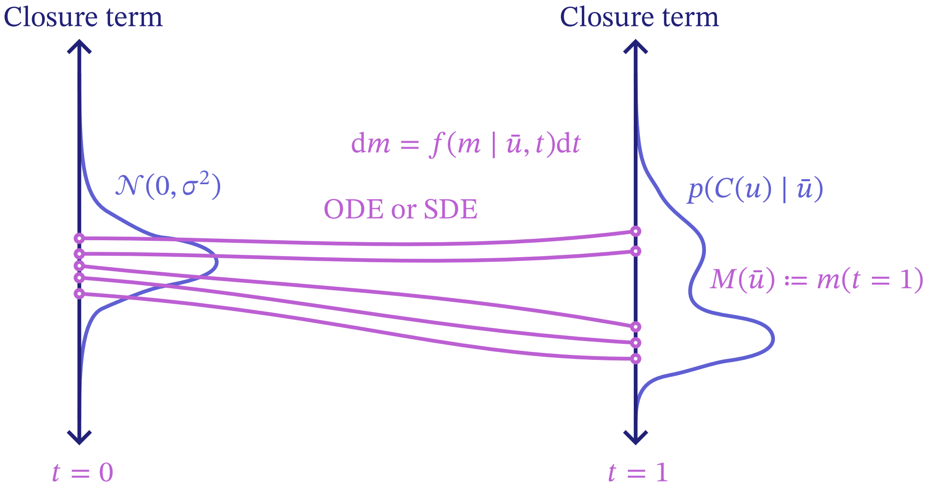

Data-driven sampling

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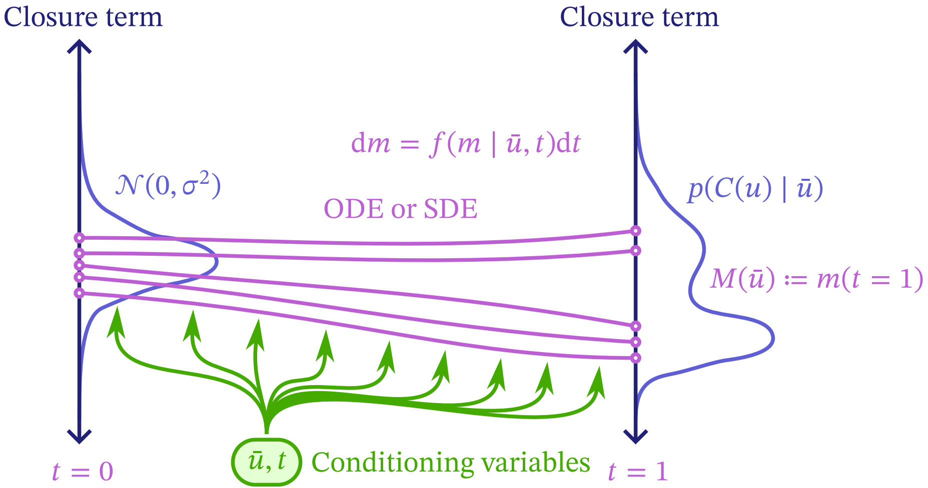

Conclusion and outlook

CWI

Conclusion and outlook

Conclusion

- Data-driven closure requires correct data
- “Discretize first” gives consistent data from DNS
- An optimal LES closure should be probabilistic
- Building probabilistic models ad-hoc can be useful, but cumbersome
- Probabilistic models can be learned with modern generative modeling

Outlook

- Merge probabilistic description of turbulence with modern generative modeling
- Velocity gradient tensor modeling

References

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