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Centrum Wiskunde & Informatica

March 4, 2026

Symmetry-preserving LES

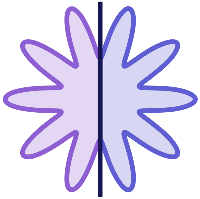
Comparison of data-driven closure models

In collaboration with Benjamin Sanderse and Roel Verstappen

This talk

Based on:

- Syver Døving Agdestein, Roel Verstappen, and Benjamin Sanderse (July 2026). "Exact Expressions for the Unresolved Stress in a Finite-Volume Based Large-Eddy Simulation". In: *Journal of Computational Physics* 556, p. 114810. DOI: 10.1016/j.jcp.2026.114810
- Syver Døving Agdestein and Benjamin Sanderse (Mar. 2026). *Comparison of Data-Driven Symmetry-Preserving Closure Models for Large-Eddy Simulation*. DOI: 10.48550/arXiv.2603.05325. arXiv: 2603.05325 [math]

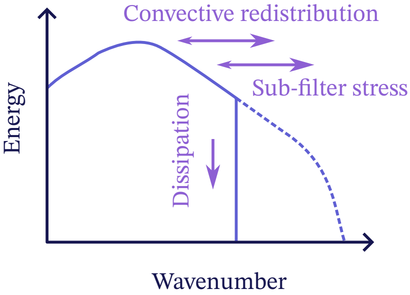


Data-driven large-eddy simulation

Turbulence and simulation

Turbulent flows are present in many engineering and natural systems.

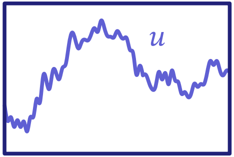
- Direct numerical simulation (DNS) resolves all scales $\Rightarrow$ cost $\sim \mathrm{Re}^{9/4}$ grid points
- Reynolds-averaged (RANS): cheap, but limited accuracy
- **Large-eddy simulation** (LES): resolve large scales, *model* the effect of small scales



Large-eddy simulation (LES)

Filter and close

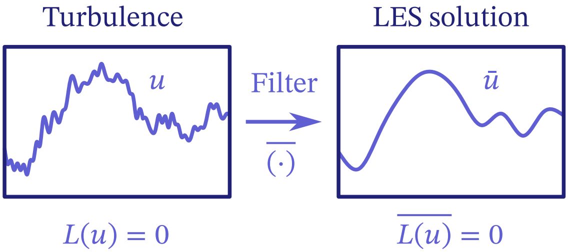
Turbulence



$$L(u) = 0$$

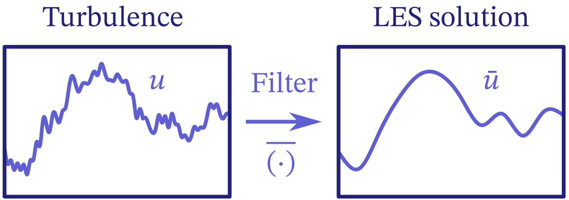
Large-eddy simulation (LES)

Filter and close



Large-eddy simulation (LES)

Filter and close

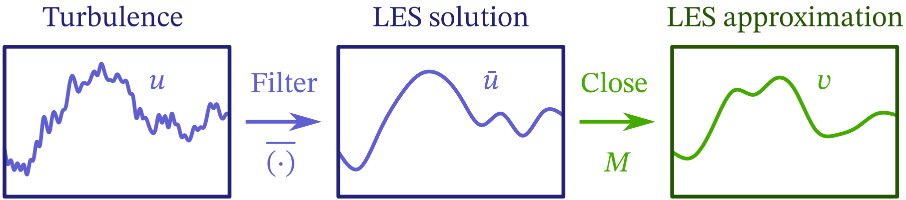


$$L(u) = 0$$

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

Large-eddy simulation (LES)

Filter and close



$$L(u) = 0$$

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

$$L(v) = -M(v)$$

The LES closure problem

Filter the incompressible Navier-Stokes equations:

$$\partial_j \bar{u}_j = 0, \quad \partial_t \bar{u}_i + \partial_j \left(\sigma_{ij}(\bar{u}) + \tau_{ij}(u) + \bar{p}\, \delta_{ij} \right) = \bar{f}_i$$

Sub-filter stress (unclosed): $\tau_{ij} := \overline{u_i u_j} - \bar{u}_i \bar{u}_j$

Closure model $m(\bar{u}) \approx \tau(u)$:

- *Functional*: match energy dissipation (e.g. Smagorinsky[1] eddy viscosity)
- *Structural*: approximate the stress tensor itself (e.g. Clark's[2] gradient model)
- *Data-driven*: learn m from DNS data using neural networks

[1] Smagorinsky 1963.
[2] Clark, Ferziger, and Reynolds 1979.

Data-driven closure

Training a neural network

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

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

A-priori (structural)

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

A-posteriori (functional)

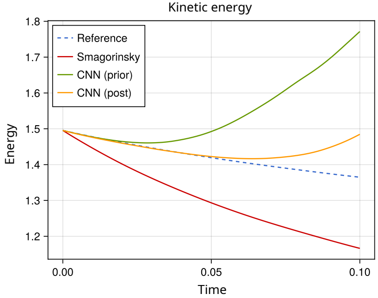
$$J_\theta(u) := \|v_\theta - \bar{u}\|^2, \quad v_\theta \text{ solution to } L(v) = -\nabla \cdot m_\theta(v).$$

Sanderse et al. 2025.

Challenge: a-priori vs. a-posteriori

Models that fit DNS data well can still be **unstable** when deployed in LES.

This work: enforce *symmetries* of the Navier-Stokes equations to improve physical consistency and stability.

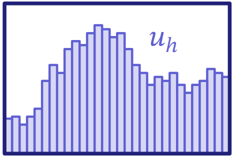


Agdestein and Sanderse 2025.

The discrete perspective

Consistent data from coarse-graining

Turbulence (DNS)

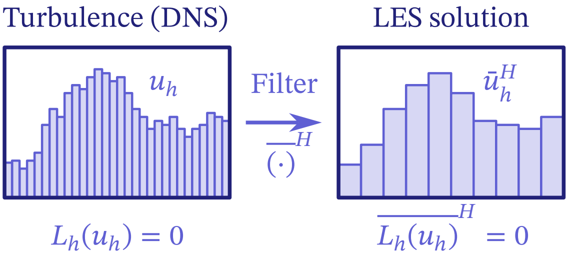


$$L_h(u_h) = 0$$

Agdestein and Sanderse 2025; Agdestein, Verstappen, and Sanderse 2026.

The discrete perspective

Consistent data from coarse-graining

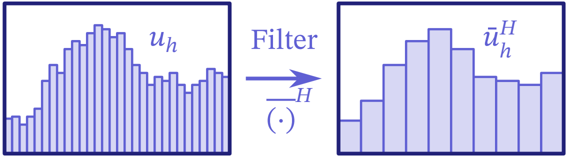


Agdestein and Sanderse 2025; Agdestein, Verstappen, and Sanderse 2026.

The discrete perspective

Consistent data from coarse-graining

Turbulence (DNS) LES solution



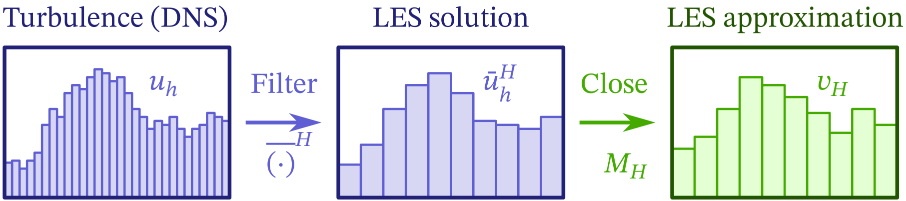
$$L_h(u_h) = 0 \qquad L_H(\bar{u}_h^H) = -C_H(u_h)$$

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

Agdestein and Sanderse 2025; Agdestein, Verstappen, and Sanderse 2026.

The discrete perspective

Consistent data from coarse-graining



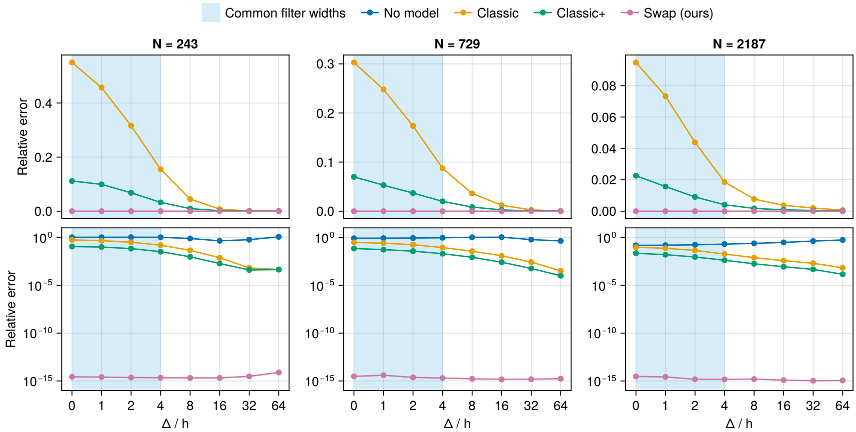
$L_h(u_h) = 0$ $\quad$ $L_H(\bar{u}_h^H) = -C_H(u_h)$ $\quad$ $L_H(v_H) = -M_H(v_H)$

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

Agdestein and Sanderse 2025; Agdestein, Verstappen, and Sanderse 2026.

The commutator expression is important

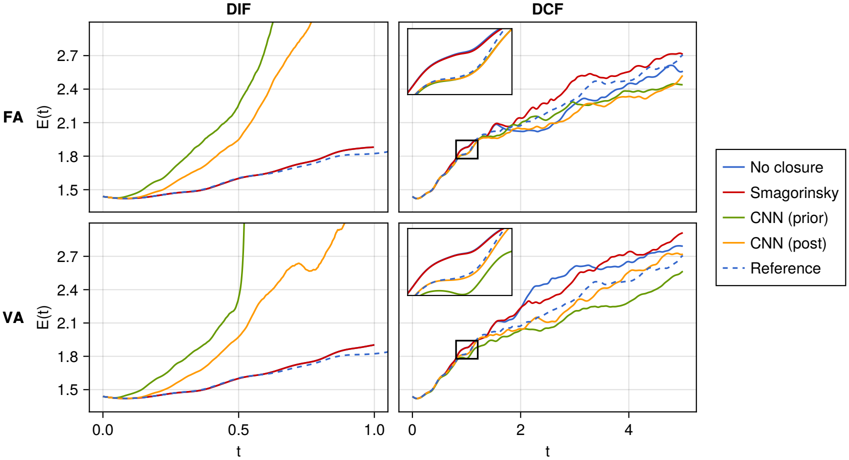
“DNS-aided LES” for Burgers’ equation



Agdestein, Verstappen, and Sanderse 2026; Bae and Lozano-Duran 2022.

The commutator expression is important

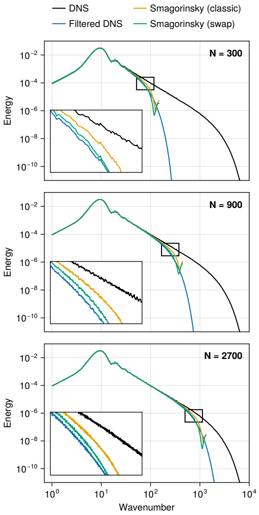
A-priori and a-posteriori learning



Agdestein and Sanderse 2025.

The commutator expression is important

Fitting a Smagorinsky model



$$S := (\nabla + \nabla^T)/2$$
$$S_H := (\nabla_H + \nabla_H^T)/2$$
$$M(\bar{u}) := -\nabla \cdot 2\theta^2 \Delta^2 |S(\bar{u})| S(\bar{u})$$
$$M_H(\bar{u}_H) := -\nabla_H \cdot 2\theta^2 \Delta^2 |S_H(\bar{u}_H)| S_H(\bar{u}_H)$$

Symmetry-preserving models

Symmetries of the Navier-Stokes equations

The incompressible Navier-Stokes equations are invariant under:

- **Galilean invariance**: $\tilde{u} = u + \dot{X}(t)$
- **Rotation invariance**: $\tilde{u}_i = Q_{ij} u_j, \; Q \in O(3)$
- **Reflection invariance**
- **Scaling invariance**: $\tilde{x} = ax$, $\tilde{u} = (a/b)\, u$, $\tilde{\nu} = (a^2/b)\, \nu$
- Pressure invariance, time translation, material frame indifference

Key insight: a closure model that violates these symmetries can introduce spurious, unphysical forces.

Oberlack 1997; Silvis, Remmerswaal, and Verstappen 2017.

Symmetry preservation in LES closures

- **Galilean invariance**: use velocity gradient tensor $\bar{A}_{ij} = \partial_j \bar{u}_i$ as input instead of $\bar{u}$
- **Scaling invariance**: use dimensionless input $\bar{A}/|\bar{A}|$ with prefactor $\Delta^2 |\bar{A}|^2$
- **Rotation/reflection**: requires special network architectures

We compare **three** neural network architectures:

1. Tensor-basis neural network (**TBNN**)
2. Group-convolutional neural network (**G-conv**)
3. Unconstrained convolutional network (**Conv**) — baseline

Tensor-basis neural network (TBNN)

Represent the closure as a linear combination of **basis tensors**:

$$m^{\text{TBNN}} = \Delta^2 |A|^2 \sum_{k=1}^{7} \alpha_k(\lambda)\, T^{(k),\text{dev}}(A^*)$$

- $T^{(k)}$: tensor basis from Smith's analysis[1] — 7 tensors, minimal and complete
- $\lambda_1, \dots, \lambda_5$: scalar invariants of S and W
- $\alpha_k = \text{NN}(\lambda_1, \dots, \lambda_5)$: standard feedforward network

Key advantage: equivariance is guaranteed by the basis — *no constraints* on the neural network architecture.

[1] Ling, Kurzawski, and Templeton 2016; Pope 1975; Smith 1971; Stallcup, Kshitij, and Dahm 2022.

Smith's tensor basis

$$
\begin{aligned}
T^{(0)} &= I, & T^{(4)} &= SW - WS, \\
T^{(1)} &= S, & T^{(5)} &= \mathbf{WSW}, \\
T^{(2)} &= S^2, & T^{(6)} &= S^2W - WS^2, \\
T^{(3)} &= W^2, & T^{(7)} &= WSW^2 - W^2SW.
\end{aligned}
$$

where $S := (A + A^T)/2$ is the strain rate and $W := (A - A^T)/2$ is the rotation rate.

Five scalar invariants:

$$\lambda_1 = \operatorname{tr}(S^2), \quad \lambda_2 = \operatorname{tr}(W^2), \quad \lambda_3 = \operatorname{tr}(S^3), \quad \lambda_4 = \operatorname{tr}(SW^2), \quad \lambda_5 = \operatorname{tr}(S^2W^2)$$

Both $T^{(k)}$ and λ transform correctly under $O(3)$
$\Rightarrow m^{\text{TBNN}}$ is automatically equivariant.

Smith 1971; Spencer and Rivlin 1958; Stallcup, Kshitij, and Dahm 2022.

Group-convolutional neural network (G-conv)

Enforce equivariance through the **network architecture**:

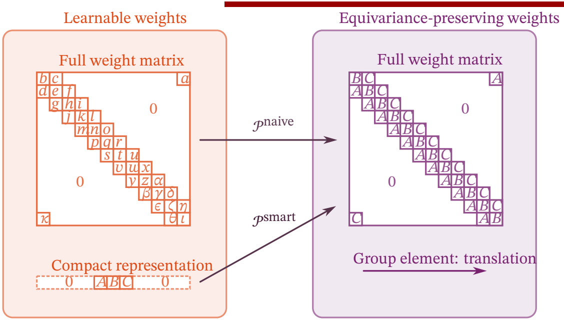
$$m^{\text{G-conv}}(\bar{u}) = \Delta^2 |\bar{A}|^2 \, \ell_n^{\mathcal{P}} \circ \cdots \circ \ell_1^{\mathcal{P}}(\bar{A}/|\bar{A}|)$$

- Symmetry group: octahedral group G ($|G| = 48$ elements: rotations by $\pi/2$ and reflections along grid axes)
- Hidden layers use the **regular representation** $\mathbb{R}^{48}$: group acts by permutation
- Weight projection: $w = \sum_{g \in G} P_g^{-1} \tilde{w} P_g$ ensures $P_g w = w P_g$

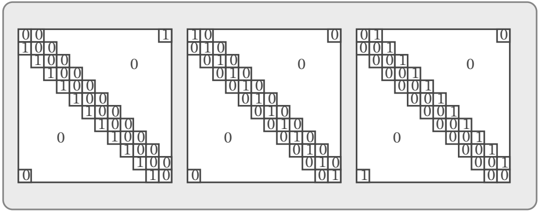
Novel contribution: eigendecomposition-based weight sharing reduces learnable parameters from 48^2 to 48 per hidden layer.

Cohen and Welling 2016.

Weight projection mechanism



Eigenvectors of $\mathcal{P}^{\text{naive}}$ with non-zero eigenvalues

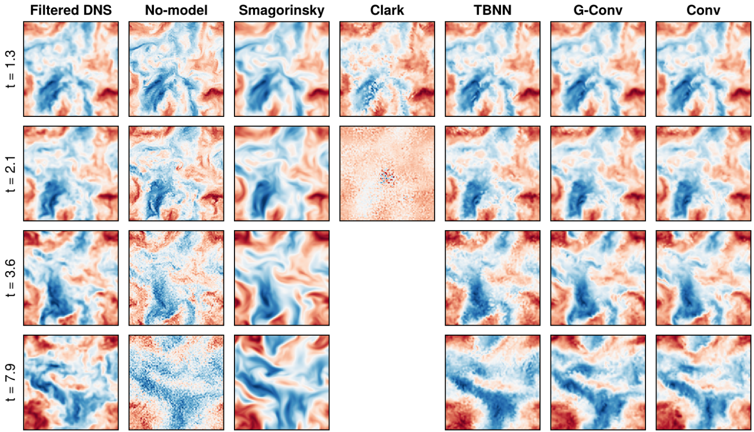


Results

Experimental setup

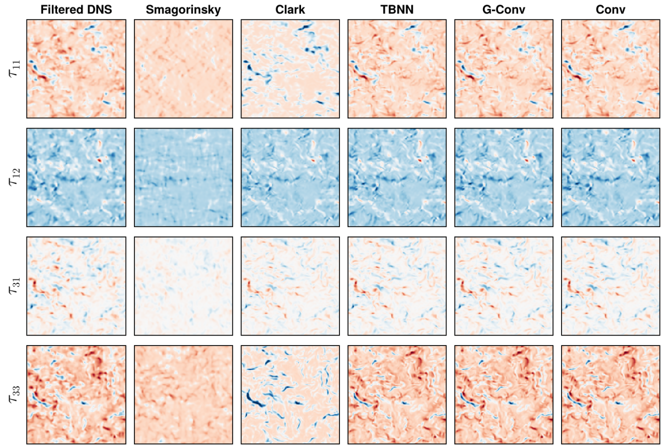
- **Flow**: forced homogeneous isotropic turbulence in $\Omega = [0, 2\pi]^3$
- **Discretization**: pseudo-spectral (DNS and LES)
- **Classical baselines**: No-model, Smagorinsky ($C_s = 0.17$), Clark
- **Data-driven models**: TBNN, G-conv, Conv (same number of trainable parameters)
- **Training**: a-priori loss, discretization-consistent targets
- **Evaluation**: a-priori (tensor prediction) and a-posteriori (LES simulation)

A-posteriori velocity fields



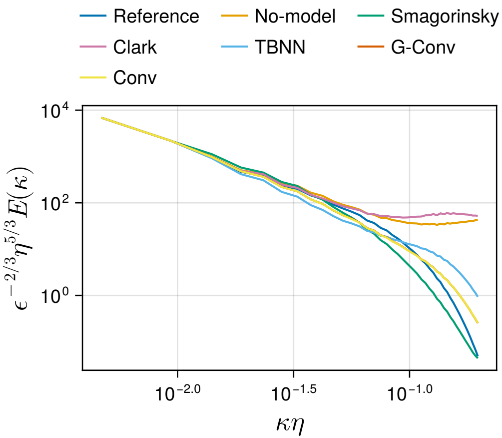
2D section of u_3 at various times. No-model and Clark amplify small-scale noise; Smagorinsky is too smooth.

A-priori stress prediction



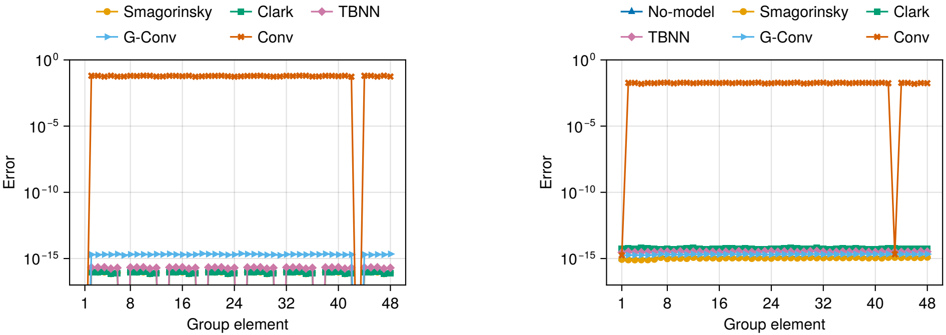
All structural closures visually resemble the reference SFS. Smagorinsky does not (it is a functional model).

Energy spectra



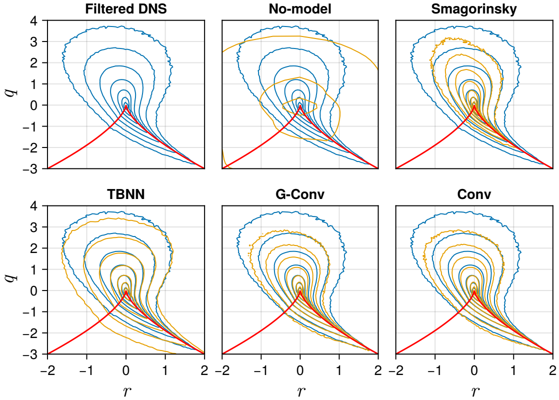
- No-model, Clark, TBNN: energy pile-up at high wavenumbers
- Smagorinsky: overly dissipative
- **Conv, G-conv**: best match to filtered DNS spectrum

Equivariance errors



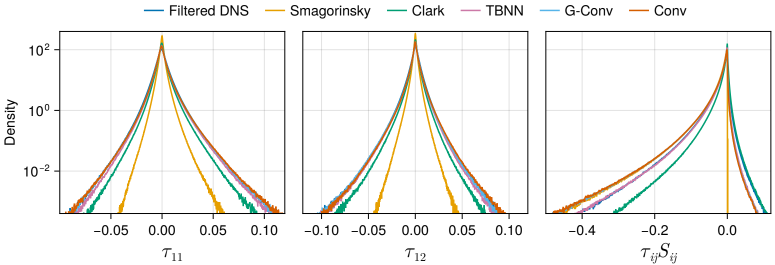
- TBNN, G-conv: equivariance errors at **machine precision**
- Conv: 5.8% a-priori error — does *not* learn equivariance from isotropic data alone

Velocity-gradient invariant distributions



The (q, r)-distribution characterizes local flow topology. Symmetry-preserving models (TBNN, G-conv) produce more physically consistent distributions than Conv.

Tensor and dissipation distributions



TBNN captures forward transfer well; Conv/G-conv are overly dissipative. Clark captures backscatter but lacks forward dissipation.

Computational cost

- G-conv is $\sim 7\times$ slower than Conv at inference (due to 48-channel regular representation)
- TBNN has inference cost **comparable to Conv**
- TBNN only predicts 7 scalar coefficients $\Rightarrow$ could use a smaller network, further reducing cost

TBNN: best trade-off between symmetry preservation and computational efficiency.

Conclusion and outlook

Conclusion and outlook

Conclusion

- For structural models, discretization-informed target data is important
- Data-driven closures **outperform** classical closures in both a-priori and a-posteriori metrics
- Unconstrained Conv achieves comparable *prediction errors* but does not learn equivariance from data alone (5.8% equivariance error)
- Symmetry-preserving models produce more consistent **velocity-gradient statistics**
- TBNN achieves equivariance at **low computational cost**; G-conv is 7× slower
- Clark is accurate at short times but **unstable** without sufficient dissipation

Outlook

- **Reynolds number generalization**: current models are trained at a single Re — can symmetry constraints improve out-of-distribution robustness?
- **Anisotropic flows**: rotational equivariance may be overly constraining near walls; relaxed group convolutions could help
- **Spatial context**: extend from pointwise to convolutional stencils or graph-based architectures

CWI

Symmetry

S. D. Agdestein

References I

Agdestein, Syver Døving and Benjamin Sanderse (Feb. 2025). "Discretize First, Filter next: Learning Divergence-Consistent Closure Models for Large-Eddy Simulation". In: *Journal of Computational Physics* 522, p. 113577. DOI: 10.1016/j.jcp.2024.113577.

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Symmetry

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Thank you!