A generative model for large eddy simulation closure modeling

NHR4CES workshop: Machine Learning in Computational Fluid Dynamics

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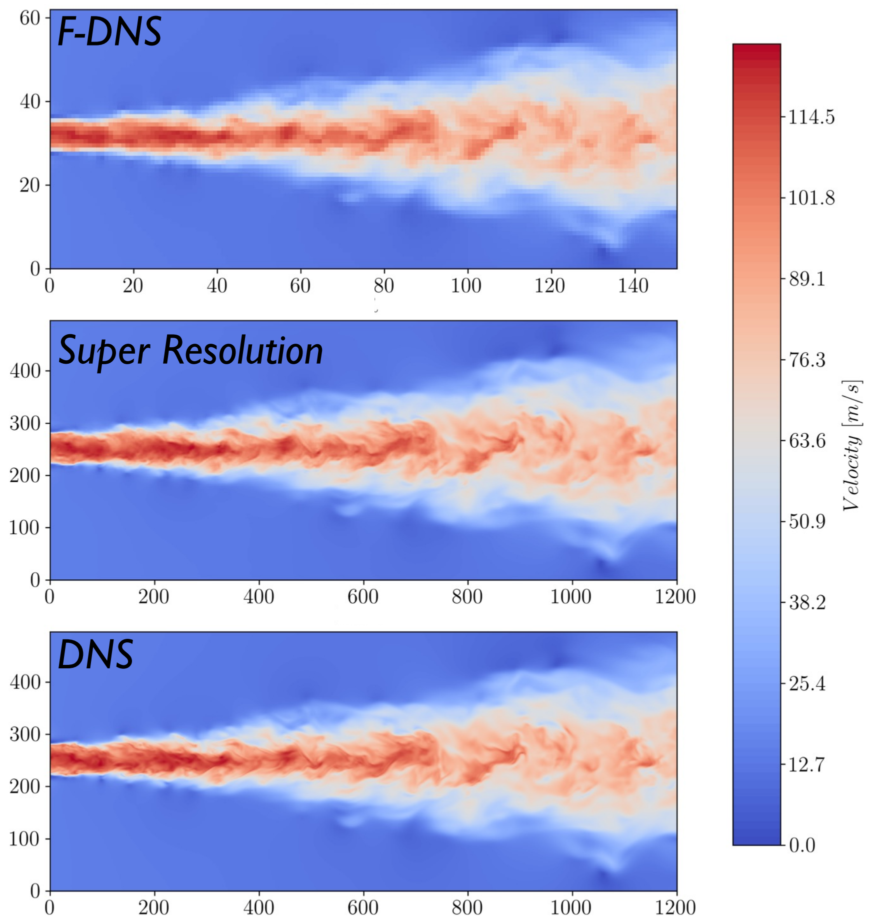


itv | RWTH AACHEN UNIVERSITY

Data-driven closure modeling

Large Eddy Simulation and closure modeling in turbulent combustion

$$\frac{\partial \bar{\rho}\widetilde{u}_j}{\partial t} + \frac{\partial \bar{\rho}\,\widetilde{u}_i\,\widetilde{u}_j}{\partial x_i} = -\frac{\partial \bar{p}}{\partial x_j} + \frac{\partial \bar{\tau}_{ij}}{\partial x_i} - \frac{\partial \boxed{\bar{\rho}\tau_{ij}^r}}{\partial x_i}$$

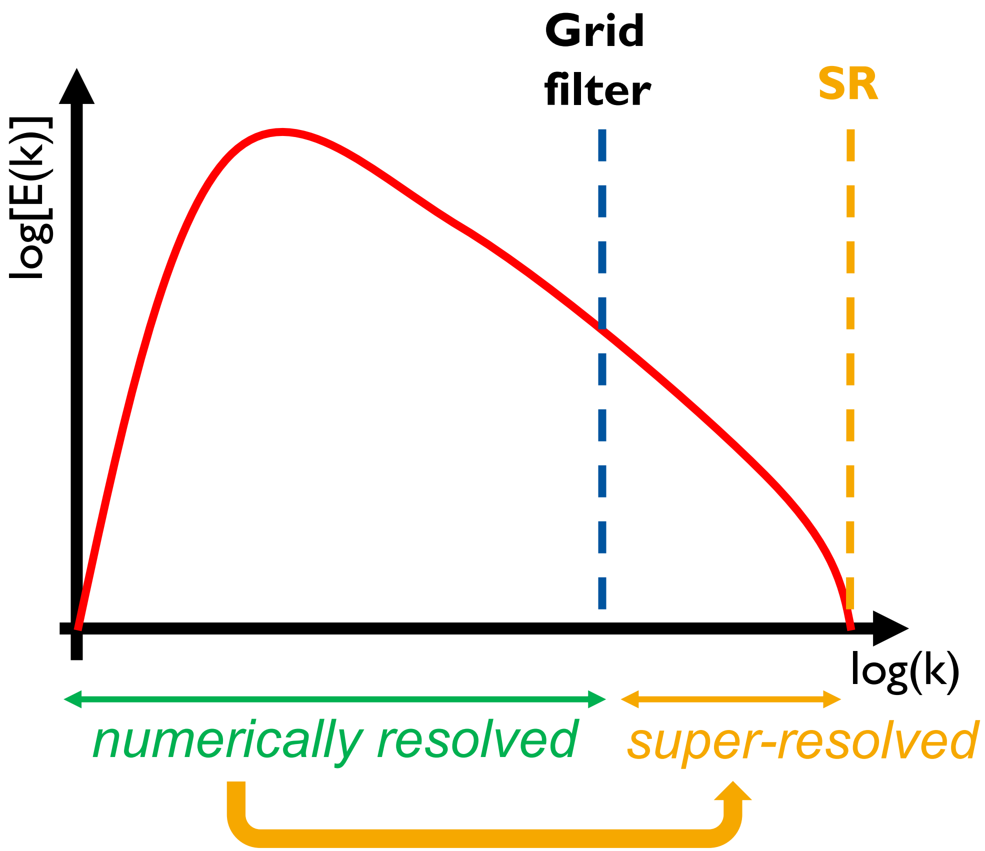
$$\frac{\partial \bar{\rho}\widetilde{\Psi}_k}{\partial t} + \frac{\partial \bar{\rho}\,\widetilde{u}_j\widetilde{\Psi}_k}{\partial x_i} = -\frac{\partial \boxed{\bar{\rho}\tau_j^T}}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\bar{\rho}D_k\frac{\partial \widetilde{\Psi}_k}{\partial x_j}\right) + \overline{\dot{\Phi}_k}$$

- **algebraic**: e.g., Smagorinsky model

$$\tau_{ij}^r \approx -2\nu_T\tilde{S}_{ij}$$

- **data-driven:** through **super-resolution**

$$\tau_{ij}^r = \widetilde{u_i\,u_j} - \tilde{u}_i\,\tilde{u}_j$$



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Fukami K et al., "Super-resolution reconstruction of turbulent flows with machine learning". J Fluid Mech, 2019.

Data-driven closure modeling

Large Eddy Simulation and closure modeling in turbulent combustion

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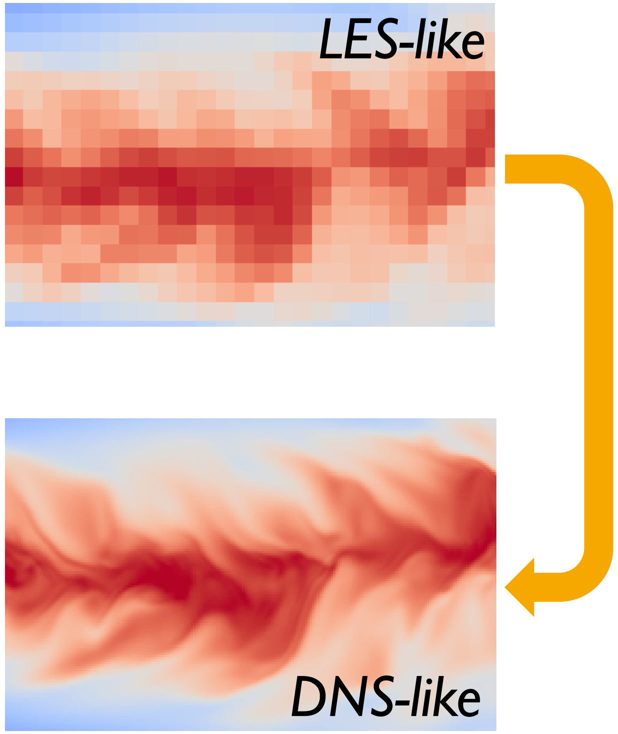


given upsampling factor

- **data-driven:** through **super-resolution**

$\tau_{ij}^{r} = \boxed{\widetilde{u_i\,u_j}} - \tilde{u}_i\,\tilde{u}_j$ *(unresolved stress tensor)*

$\tau_{j}^{T} = \boxed{\widetilde{u_j\ T}} - \tilde{u}_j\,\tilde{T}$ *(unresolved scalar flux)*

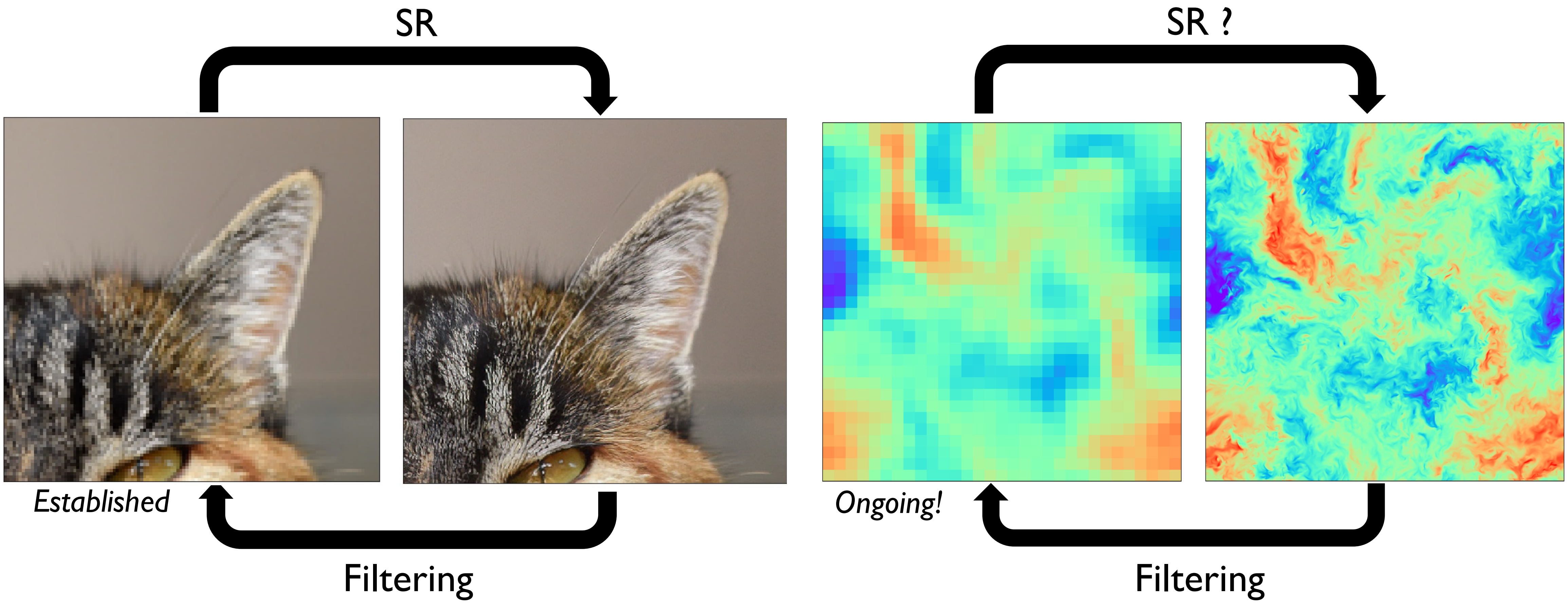
evaluated at DNS resolution

(original idea proposed by Fukami et al. and Bode et al.)

Fukami K et al., "Super-resolution reconstruction of turbulent flows with machine learning". J Fluid Mech, 2019.
M. Bode et al., "Using physics-informed enhanced super-resolution GAN for subfilter modeling in turbulent reactive flows". Proc. Combust. Inst., 2021.

Super-resolution approach for closure modeling

Could we use the super-resolution approach for subfilter-scale modeling?



C. Ledig *et. al*, "Photo-realistic single image super-resolution using a generative adversarial network". 2017 IEEE CVPR, 2017, pp. 105–114.
Nista et al., "The influence of adversarial training on turbulence closure modeling". AIAA SciTech 2022 Forum, 2022.

Outline

I. Neural network architecture and training strategy

- *Supervised vs semi-supervised approach*

II. A-priori in-sample analysis

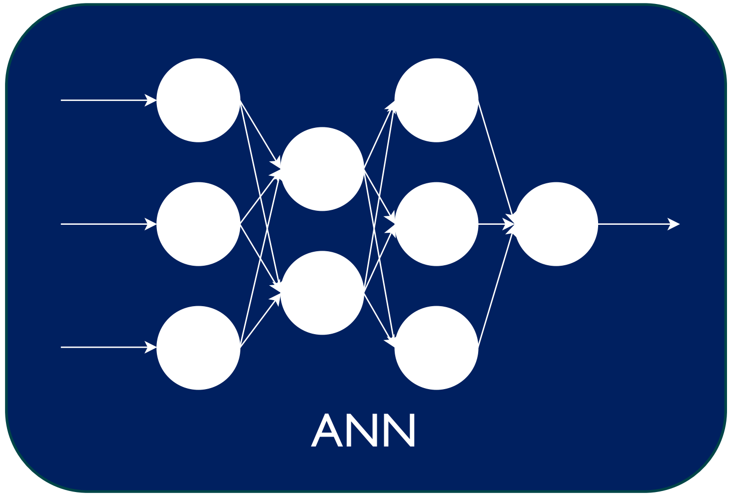
III. Generalization capability

- *at different Reynolds number*
- *on a different jet flame*
- *at different combustion regimes*
- *of the input variables*

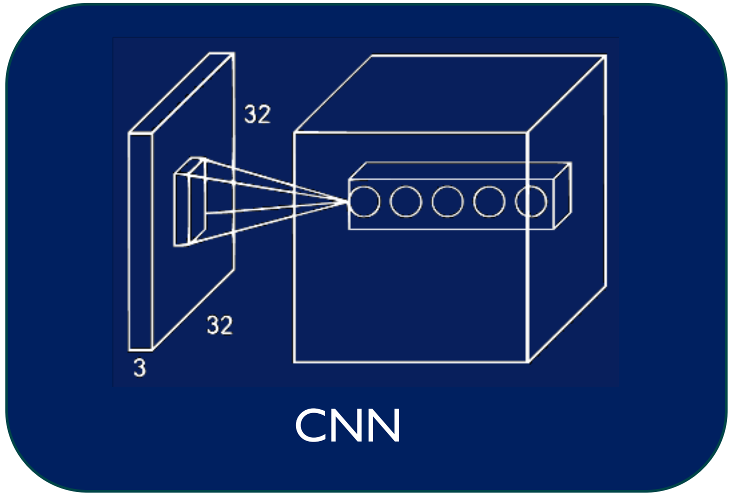
IV. Conclusion and future outlook

What architecture should we use?

Recent types of ML architectures for super-resolution subfilter-scale modeling



- simplest ML approach
- ability to work with incomplete knowledge
- **missing spatial information**

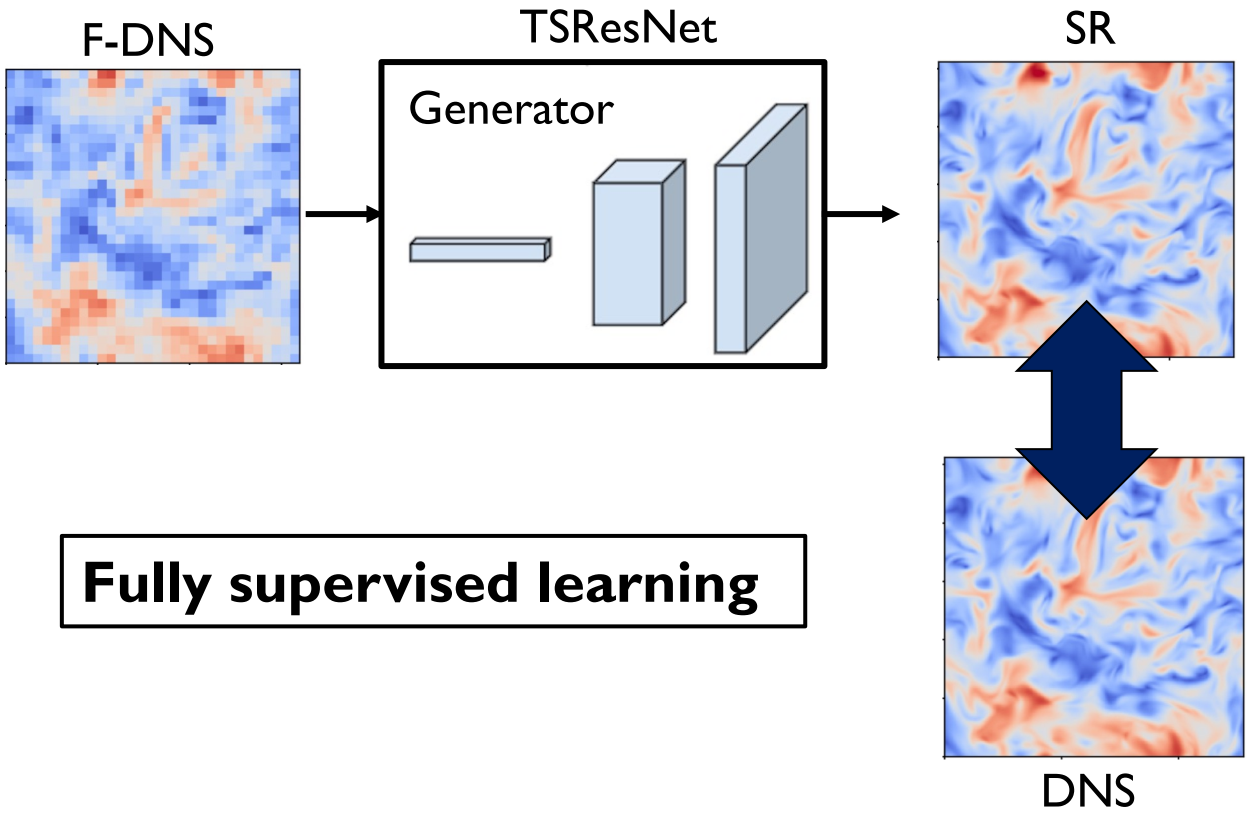


- mostly used for image recogn.
- fully connected layers
- **Several frameworks already available**

Brunton et al., "Machine learning for fluid mechanics". Annual Review of Fluid Mechanics, Vol. 52, 2020, pp. 477–508.
Goodfellow et al., "Generative adversarial networks". Communications of the ACM, Vol. 63, No. 11, 2020, pp. 139–144.

Supervised learning

TSResNet architecture



$$L_{gen} = \beta_1 L_{pixel} + \beta_2 L_{gradient} + \boldsymbol{\beta_3 L_{continuity}}$$

Fully supervised learning

This approach presents some challenges!

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Nista et al., "The influence of adversarial training on turbulence closure modeling". AIAA SciTech 2022 Forum, 2022.

What architecture should we use?

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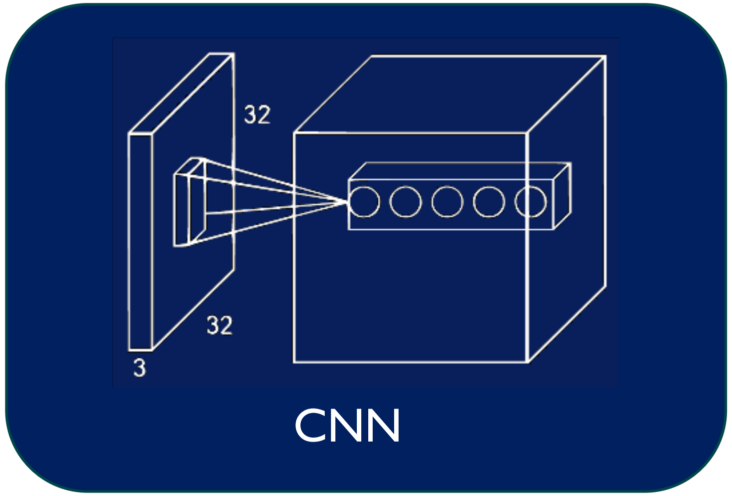

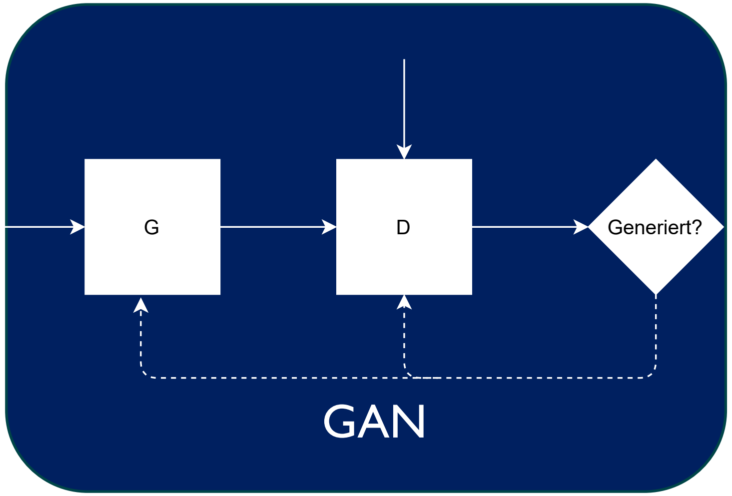

- **large amount** of data required
- lack **generalization capabilities**
- cannot guarantee **high-wavenumber details**

- **estimates PDF** of observed data
- **semi-supervised learning**
- **increases information content**

Brunton et al., "Machine learning for fluid mechanics". Annual Review of Fluid Mechanics, Vol. 52, 2020, pp. 477–508.
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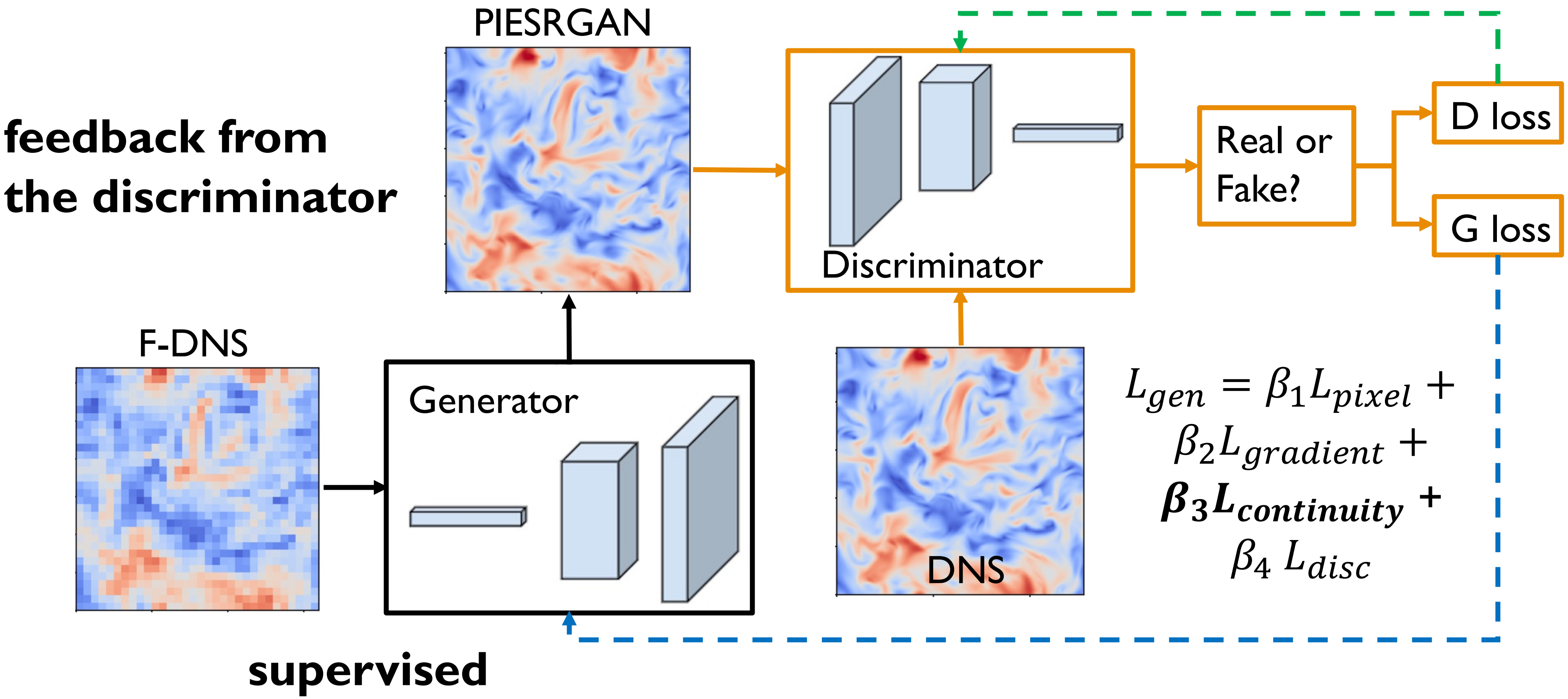
Super-Resolution Generative Adversarial Network

PIESRGAN architecture



$$L_{gen} = \beta_1 L_{pixel} + \beta_2 L_{gradient} + \boldsymbol{\beta_3 L_{continuity}} + \beta_4 L_{disc}$$

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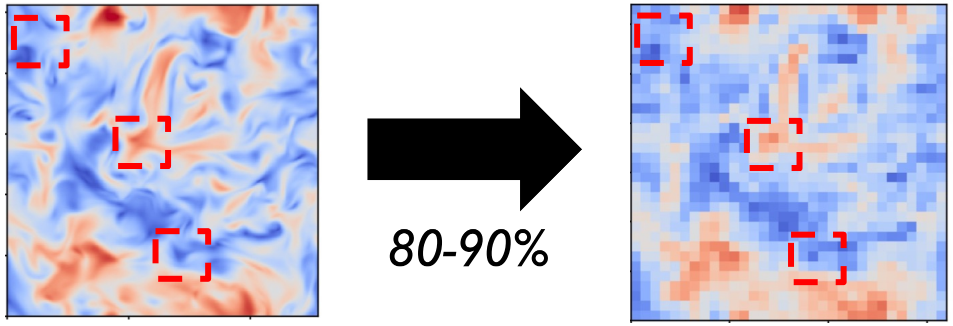
Nista et al., "The influence of adversarial training on turbulence closure modelling". AIAA SciTech 2022 Forum, 2022.

Preprocessing & training strategy

Preprocessing

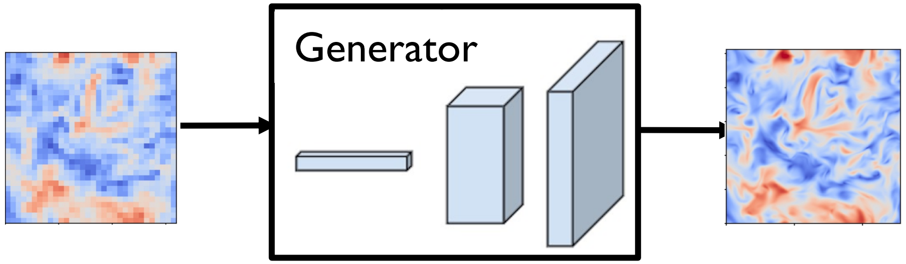
Training on a Forced HIT DNS dataset with $Re_\lambda = 88$



- <u>filtering</u> the DNS dataset (e.g. *box* or *gaussian* kernel) to obtain the input data
- <u>extracting</u> sub-boxes to be used during the training
- <u>normalizing input variables</u>: $(u, v, w) \in [0,1]$

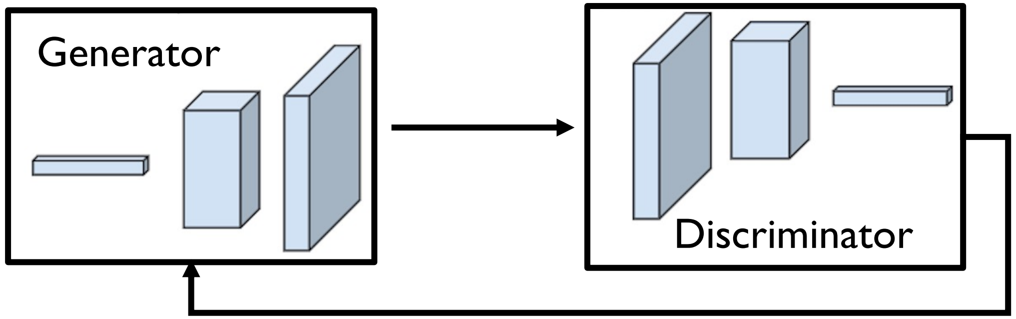
Training strategy

<u>1st training phase</u>



Supervised: *only pixel loss*

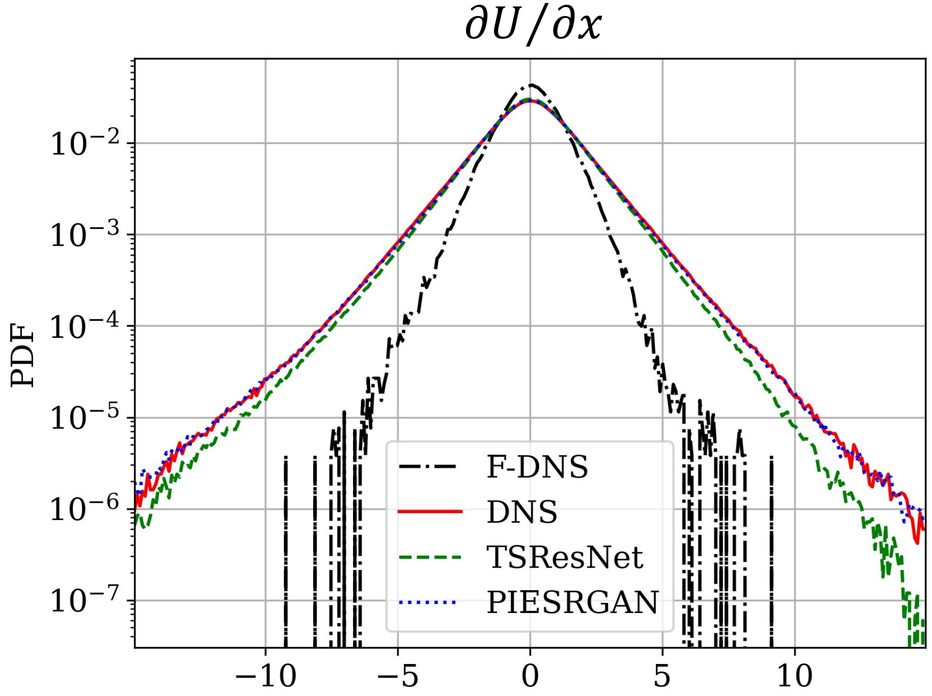
<u>2nd training phase</u>

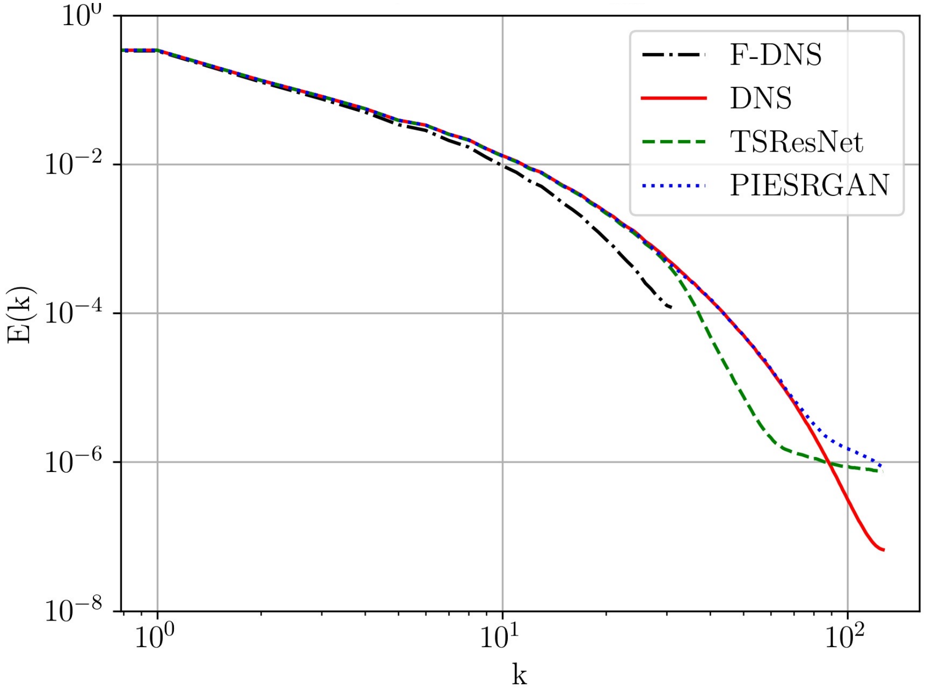


Nista et al., "The influence of adversarial training on turbulence closure modeling". AIAA SciTech 2022 Forum, 2022.
M. Gauding, "Statistics and scaling laws of turbulent scalar mixing at high Reynolds numbers". Cuvillier Verlag, 2014.

Supervised vs Semi-supervised training

PDFs of velocity gradients and energy spectra





TSResNet model captures only larger features/large scales well, while **PIESRGAN** almost exactly **predicts the DNS results** and **reproduced accurately the kinetic energy spectra** over wider spatial wavenumbers

Nista et al., "The influence of adversarial training on turbulence closure modeling". AIAA SciTech 2022 Forum, 2022.

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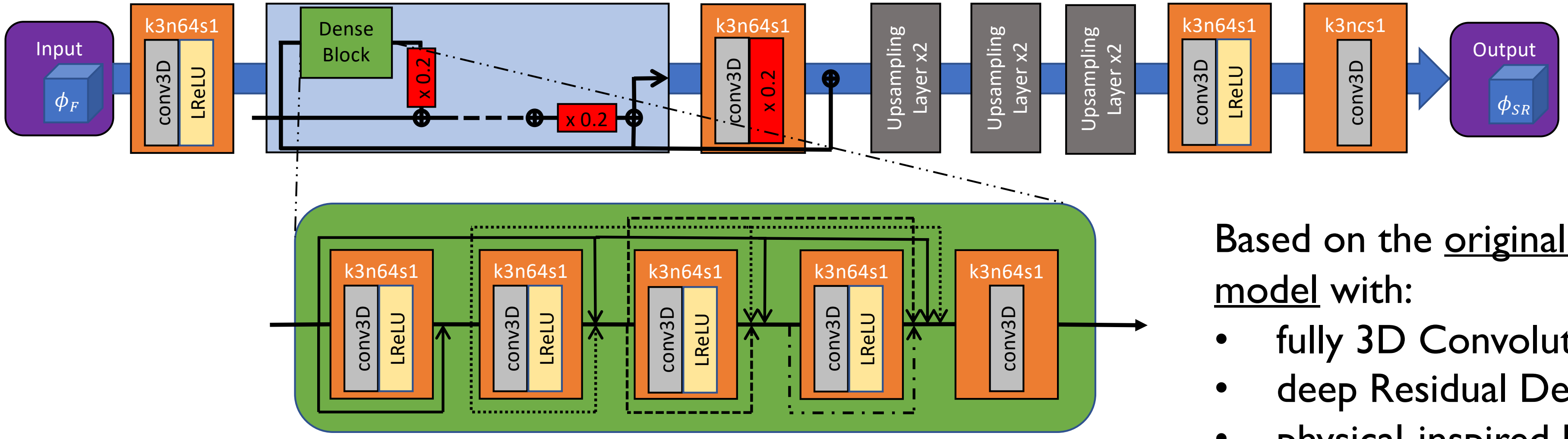
PIESGAN network structure

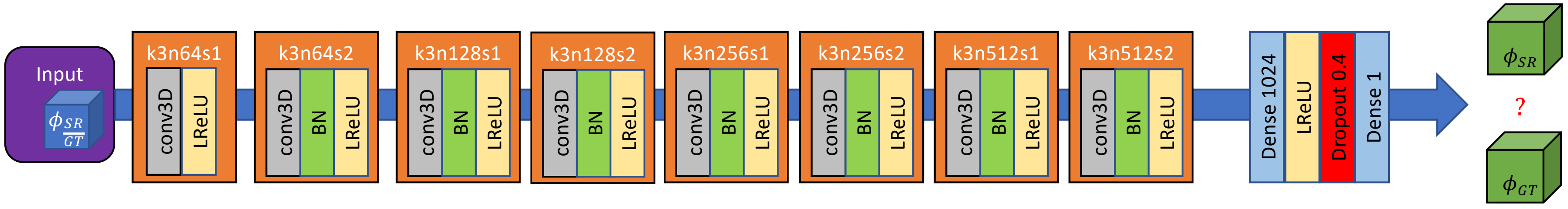
Generator



Based on the original ESRGAN model with:

- fully 3D Convolutional Layers
- deep Residual Dense Blocks
- physical-inspired Loss Function
- different upsampling layers

Discriminator



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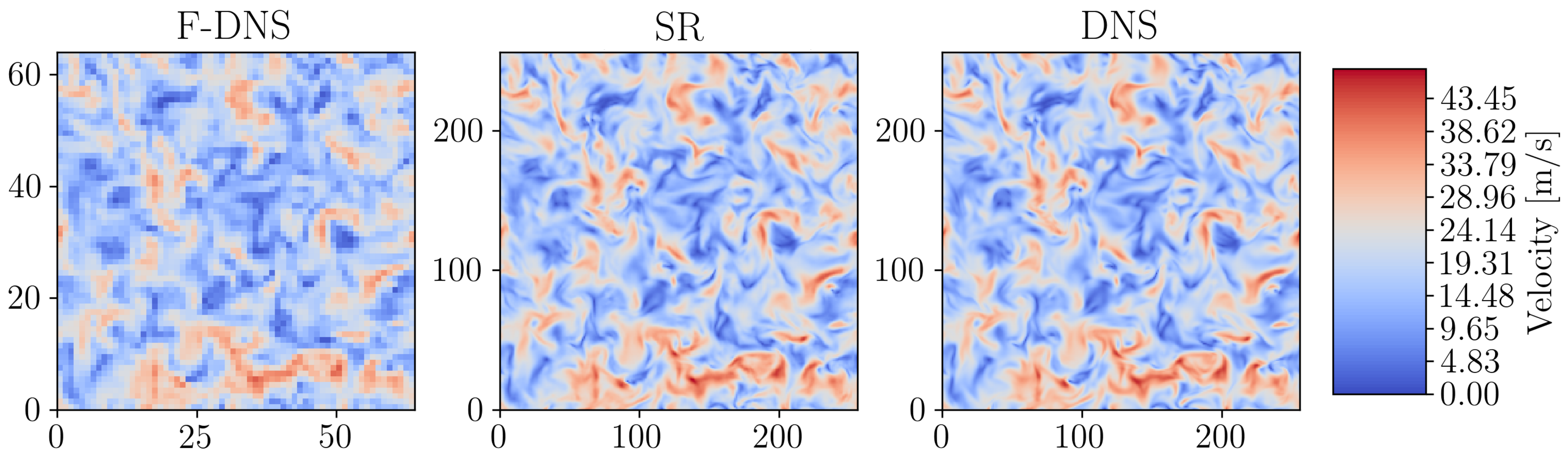
M. Bode et al., “Using physics-informed enhanced super-resolution GAN for subfilter modeling in turbulent reactive flows”. Proc. Combust. Inst., 2021.

A-priori in-sample analysis: non-reactive configuration

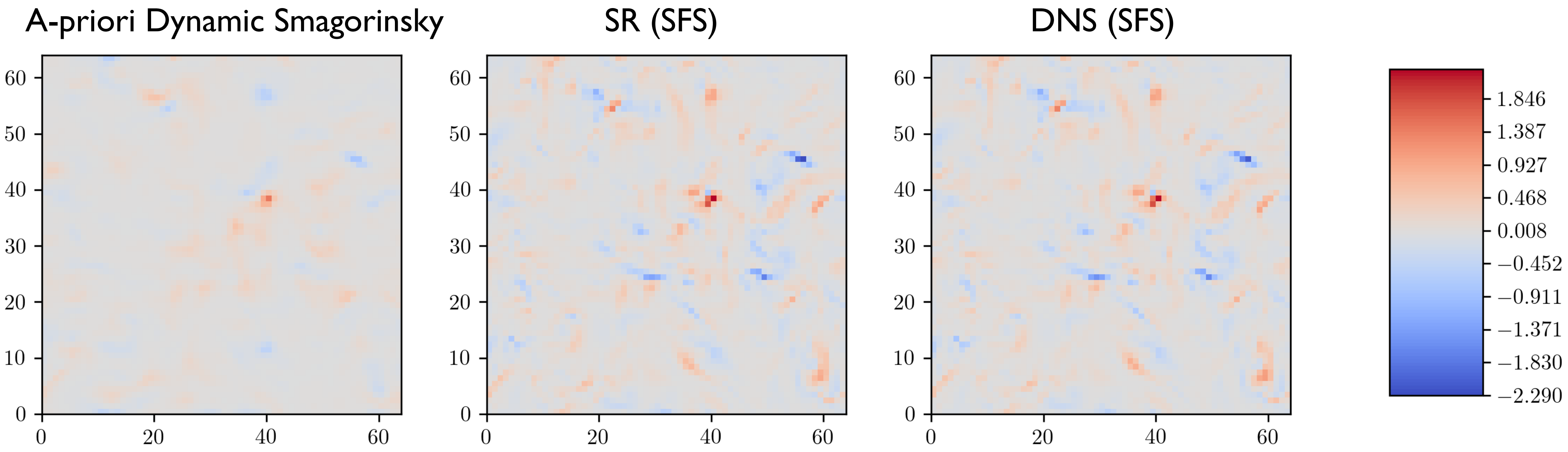
Visual similarities (velocity magnitude)



- **the GAN model** reconstructs fairly well *small-scale structures*, <u>not included in the input</u>
- at this level, **there are no visible differences**

Nista et al., "The influence of adversarial training on turbulence closure modelling". AIAA SciTech 2022 Forum, 2022.

Comparison of a-priori SFS stress tensor component τ_{11} (jPDF)



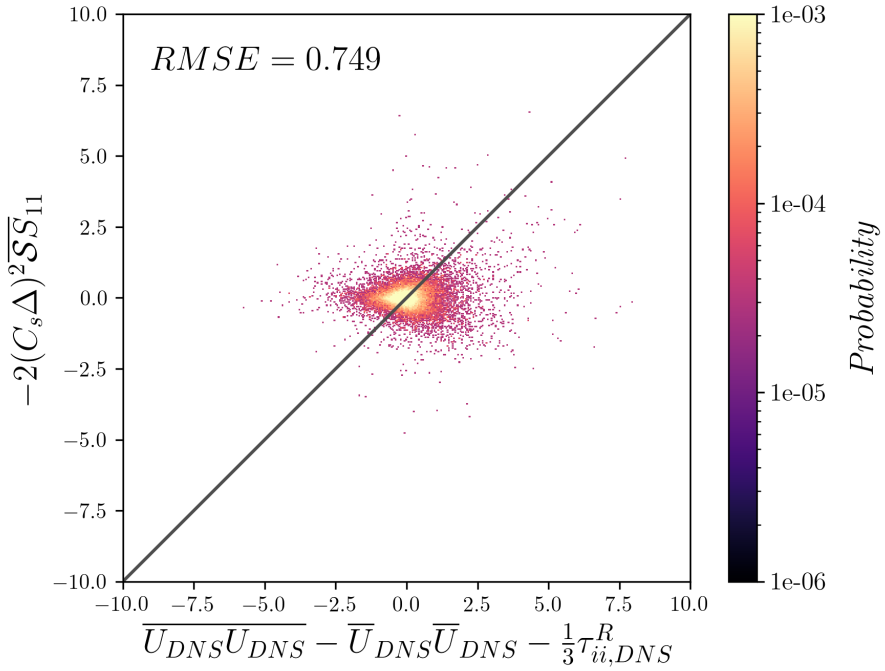
$\tau_{ij}^{r} = (C_s\Delta)^2|S|S_{ij}$ $\quad$ $\tau_{ij}^{r} = \overline{u_i u_j} - \overline{u}_i\overline{u}_j$ $\quad$ $\tau_{ij}^{r} = \overline{u_i u_j} - \overline{u}_i\overline{u}_j$

Nista et al., "The influence of adversarial training on turbulence closure modelling". AIAA SciTech 2022 Forum, 2022.

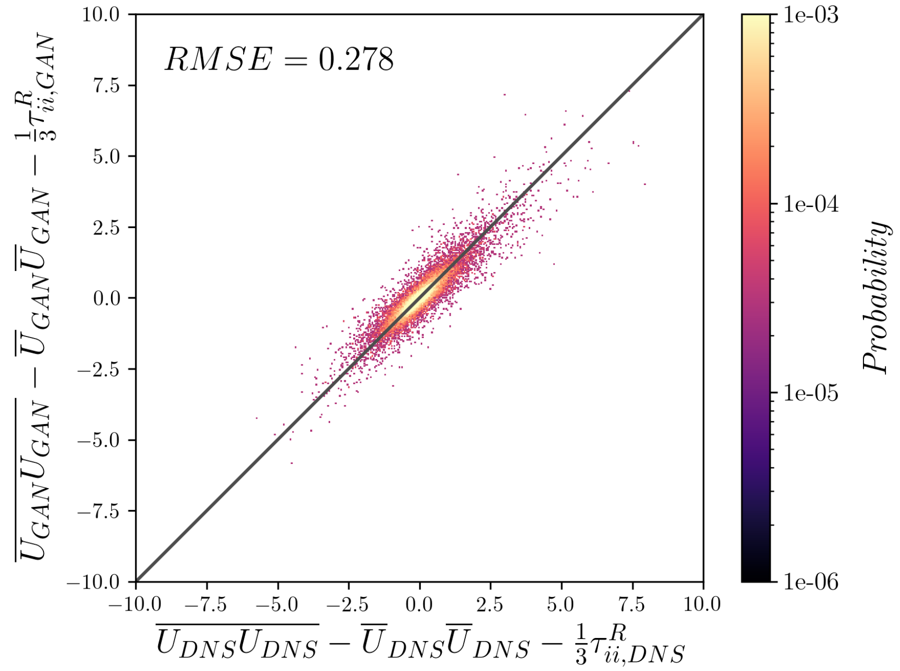
A-priori in-sample analysis: non-reactive configuration

Comparison of a-priori SFS stress tensor component τ_{11} (jPDF)

Dynamic Smagorinsky model



SR model



➢ **remarkable correlation** of the SR model with the DNS

Nista et al., "The influence of adversarial training on turbulence closure modelling". AIAA SciTech 2022 Forum, 2022.

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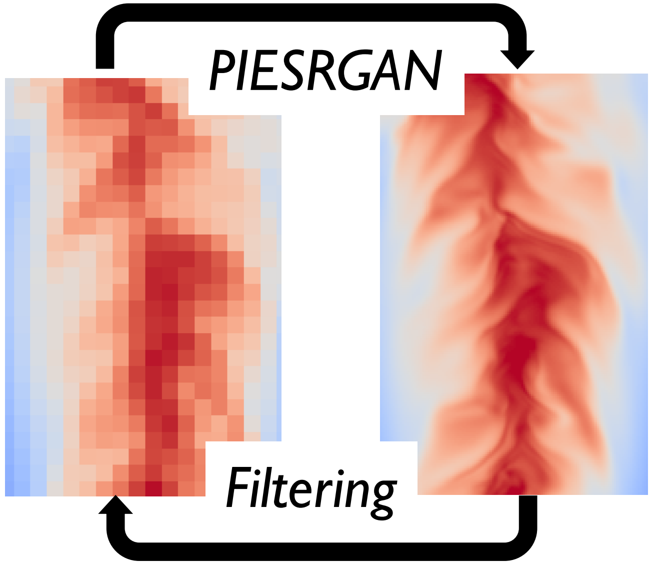
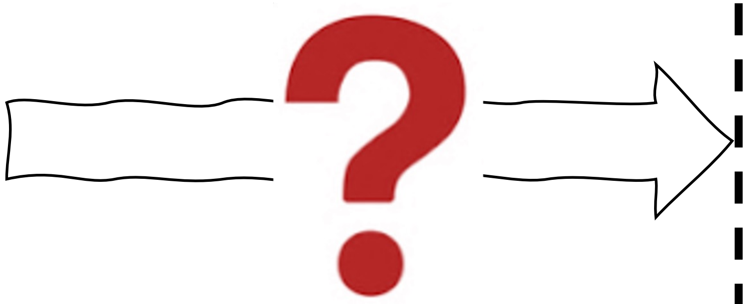
Generalization capabilities of data-driven models

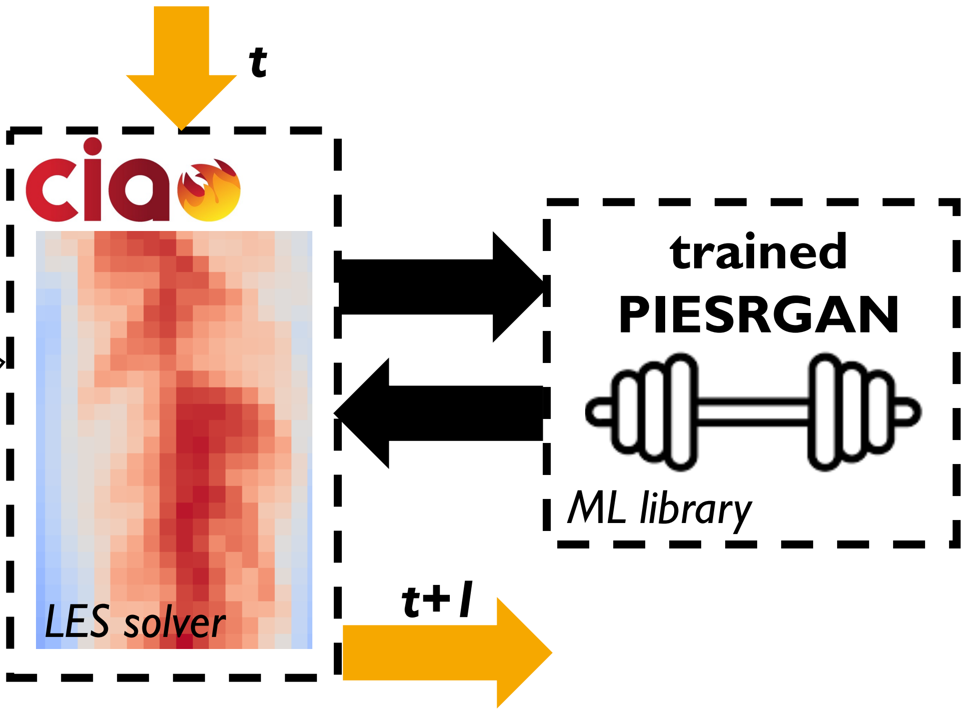
Existing challenges of data-driven models



A-priori: established



Open research issues



A-posteriori: not fully stable!

Quantify the uncertainties of ML models

Interpretably (black box nature)

Evaluation of out-of-sample predictions

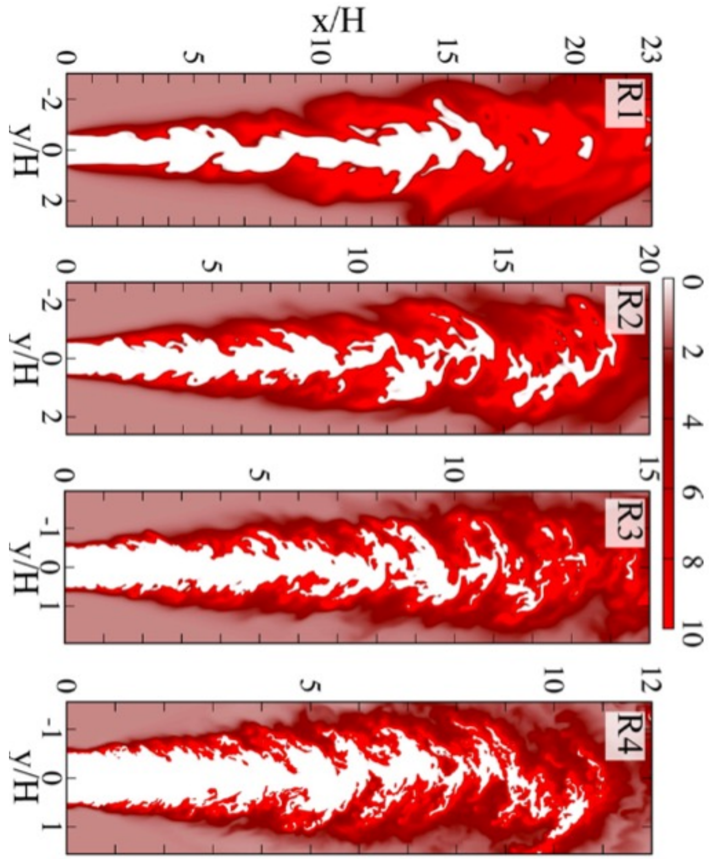
Generalization at different Reynolds numbers

Premixed methane/air jet flames DNS dataset

Phys. Param.	R1K1	R2K1	R3K1	R4K1
Re [-]	**2800**	**5600**	**11200**	**22400**
η [μm]	18	23	25	25
δ_L [μm]	110	110	110	110
dx [μm]	20	20	20	20
Ka [-]	39	23	21	21

increasing Re

roughly constant



Is the SR model learning any of those physical quantities?

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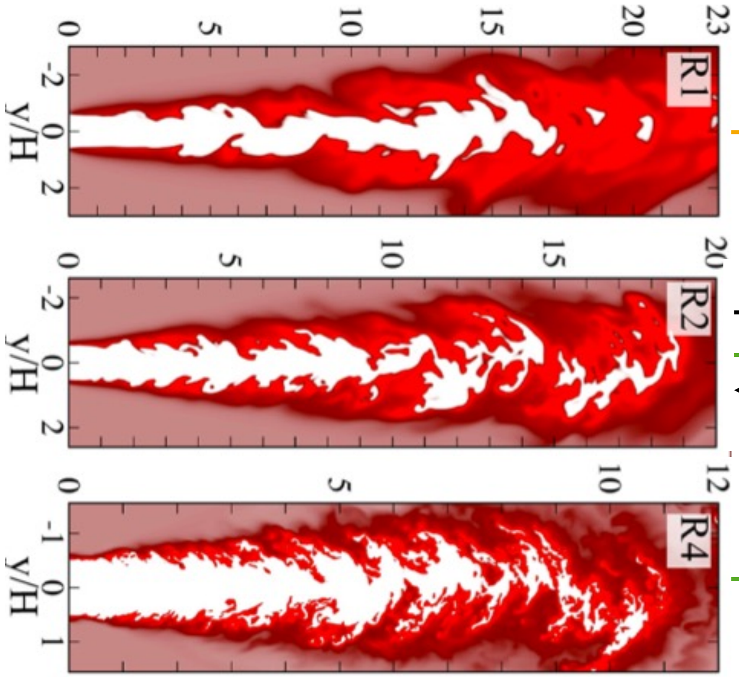
S. Luca et al., "On the statistics of flame stretch in turbulent premixed jet flames", Proc. Combust. Inst., 2018.

Generalization at different Reynolds numbers

Premixed methane/air jet flames DNS dataset



Out-of-sample prediction
Extrapolation at
lower Re

Good prediction

In-sample prediction
Same training and
testing conditions

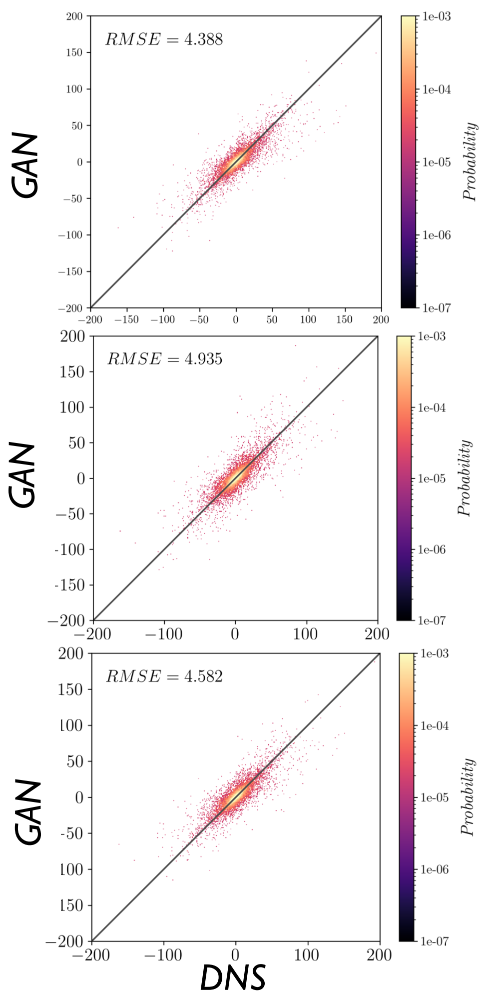
Reference model

Only R2 training

Out-of-sample prediction
Extrapolation at
higher Re

Good prediction

jPDF SFS stress τ_{12}



Good extrapolation at both lower and higher Re numbers

Is there any ratio that must be preserved between training and testing conditions to ensure generalizability?

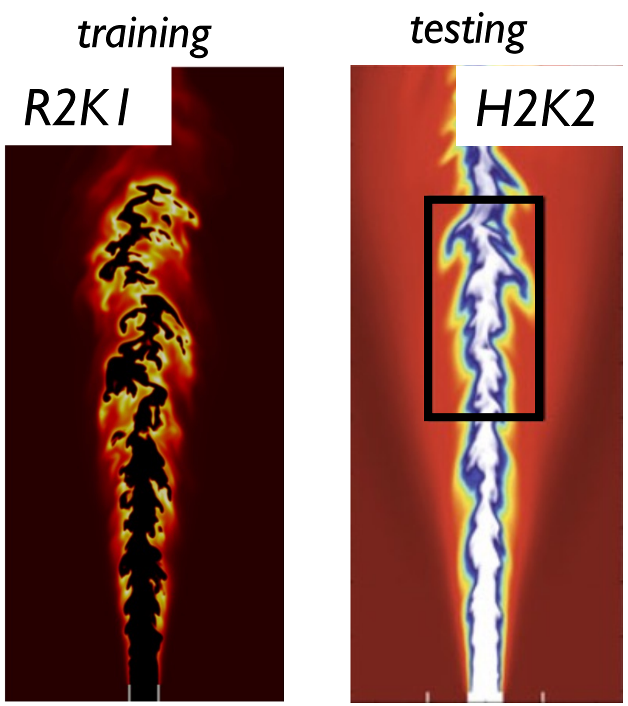
S. Luca et al., “Turbulent flame speed and reaction layer thickening in premixed jet flames”, Proc. Combust. Inst., 2018.
L. Nista et al., “Investigation of the generalization capability of a GAN for LES of turbulent premixed reacting flows”, Proc. Combust. Inst., 2022.

Generalization on a different jet flame

Generalization on a hydrogen/air jet flame

	training	*testing*
Phys. Param.	*R2K1*[1]	*H2K2*[2]
Re [-]	5600	5000
$\eta\ [\mu m]$	**23**	**10.2**
$\delta_L\ [\mu m]$	**110**	**435**
Ka [-]	23	43.5
$dx\ [\mu m]$	20	17

- Similar *Re*
- **Larger** Δ/η compared to R2K1
- **Smaller** Δ/δ_L compared to R2K1
- Similar *Ka*

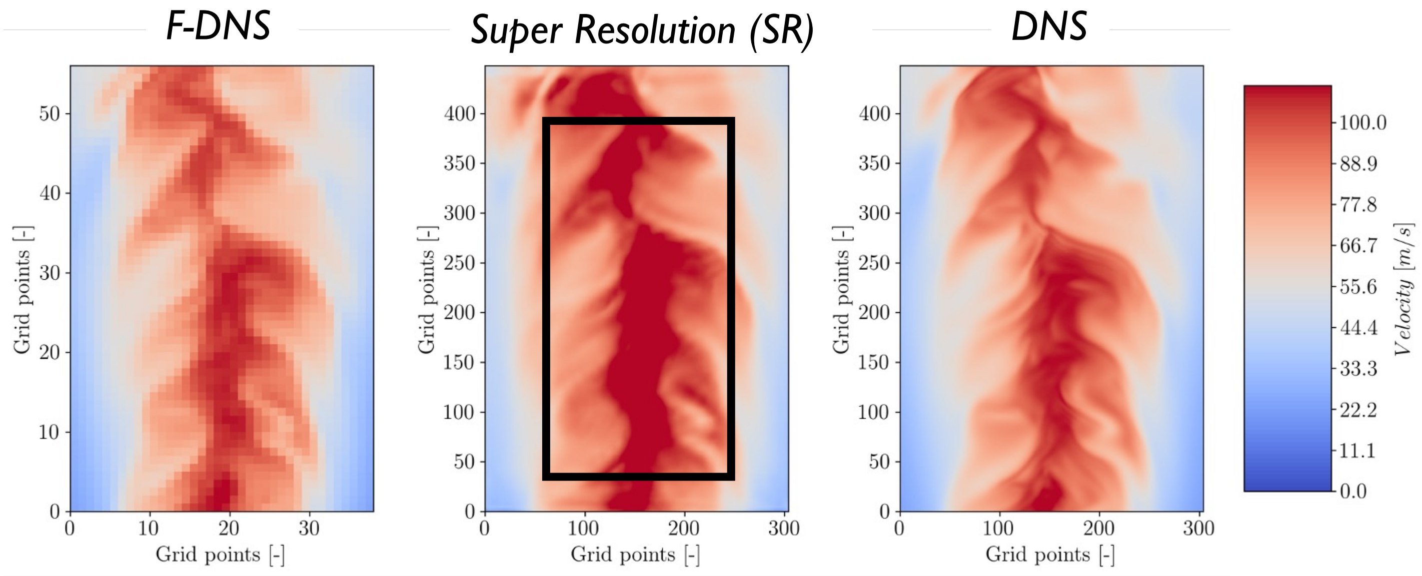


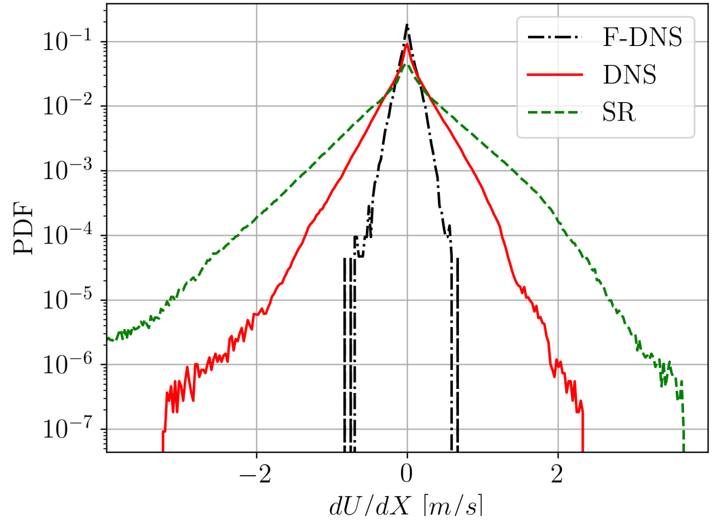
2 different approaches:
- filter size **consistent with the training:** Δ/η **and** Δ/δ_L **are not equal** to the training
- **filter size is adjusted to match** Δ/η of the training

S. Luca et al., "On the statistics of flame stretch in turbulent premixed jet flames", PROCI 2018
J. MacArt et al., "Effects of combustion heat release on velocity and scalar statistics in turbulent premixed jet flames", C&F 2018

Generalization on a different jet flame

Fs consistent with the training



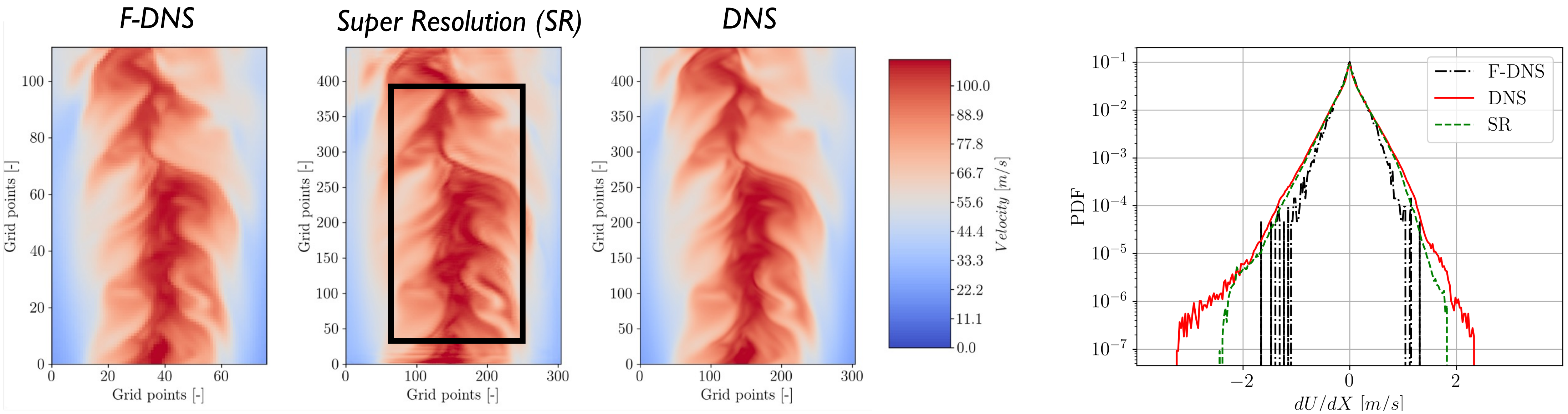


- ➢ **strong overprediction of the velocity in the jet region** which results in thicker and without small-scales turbulent oscillations
- ➢ **the error is less marked in the coflow**

L. Nista et al., "Investigation of the generalization capability of a GAN for LES of turbulent premixed reacting flows", Proc. Combust. Inst., 2022.

Generalization on a different jet flame

Fs rescales to match $^{\Delta}/_{\eta}$ - adjusting the input field



➢ **SR field looks visibly sharper**, where some features at the jet regions are enhanced

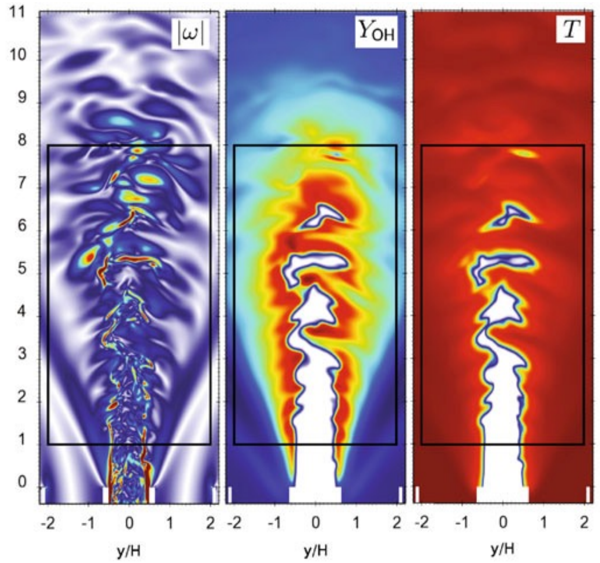
The **ratio** between the **Kolmogorov scale and grid size** must be preserved between training and testing **to ensure generalization**

L. Nista et al., "Investigation of the generalization capability of a GAN for LES of turbulent premixed reacting flows", Proc. Combust. Inst., 2022.

Generalization at different combustion regimes

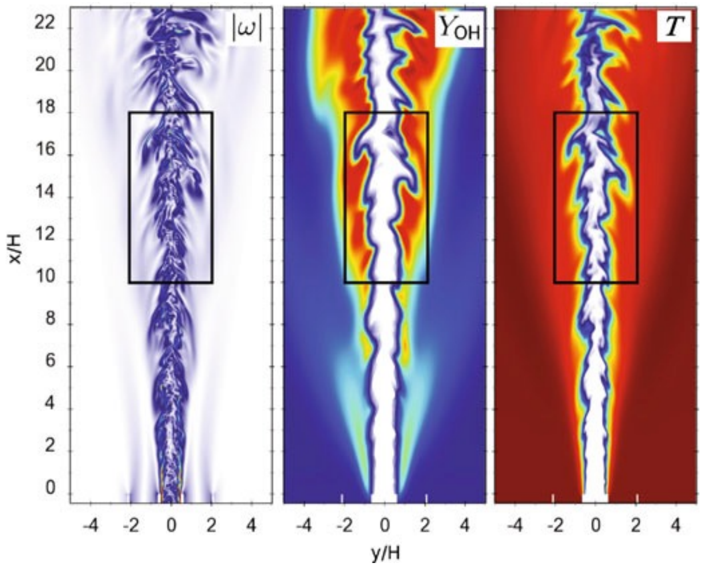
Phys. Param.	H2K1	H2K2
Re [-]	5000	5000
U [m/s]	23	93
Ka [-]	**2.6**	**32**
u'/S_L [-]	1.25	7.0
η [μm]	40	10
δ_L [μm]	435	435

$Ka < Ka_{cr}$ **(Low Ka)**



Heat release **strongly** affects vorticity

$Ka > Ka_{cr}$ **(High Ka)**



Heat release **barely** affects vorticity

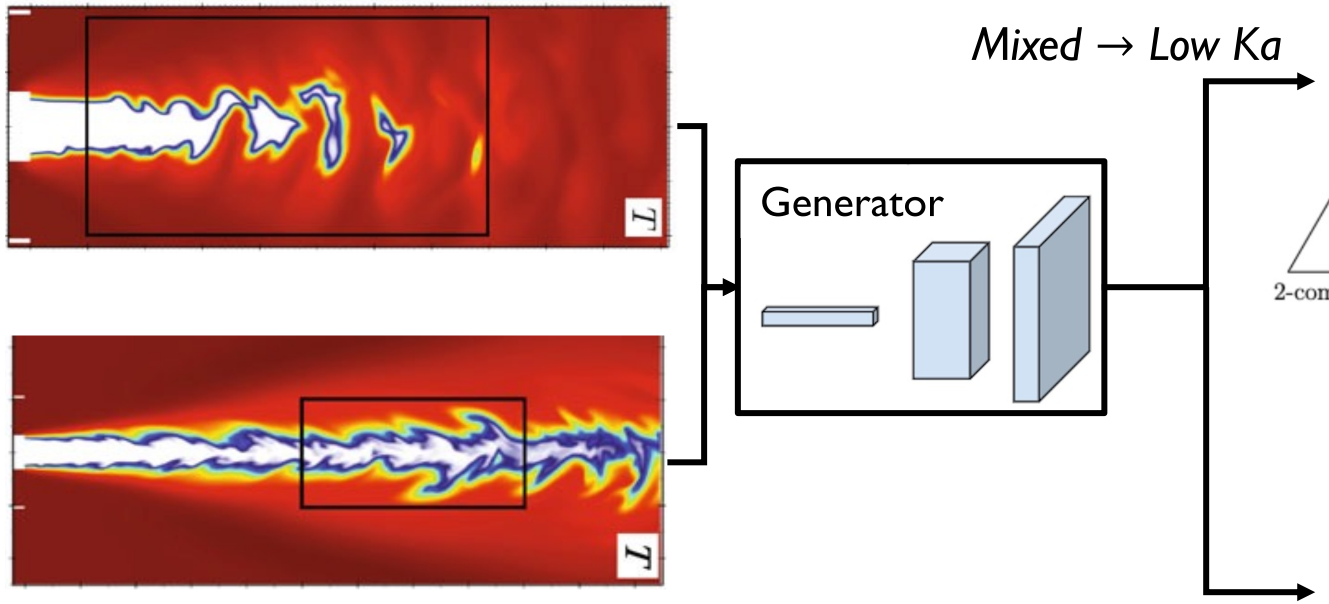
Strong influence of heat release on turbulence below the critical Karlovitz number

J. MacArt et al., “Effects of combustion heat release on velocity and scalar statistics in turbulent premixed jet flames”, Combustion and Flame, 2018
T. Grenga et al., “Predictive data-driven model based on generative adversarial network for premixed turbulence-combustion regimes”, CST, 2020

Generalization at different combustion regimes

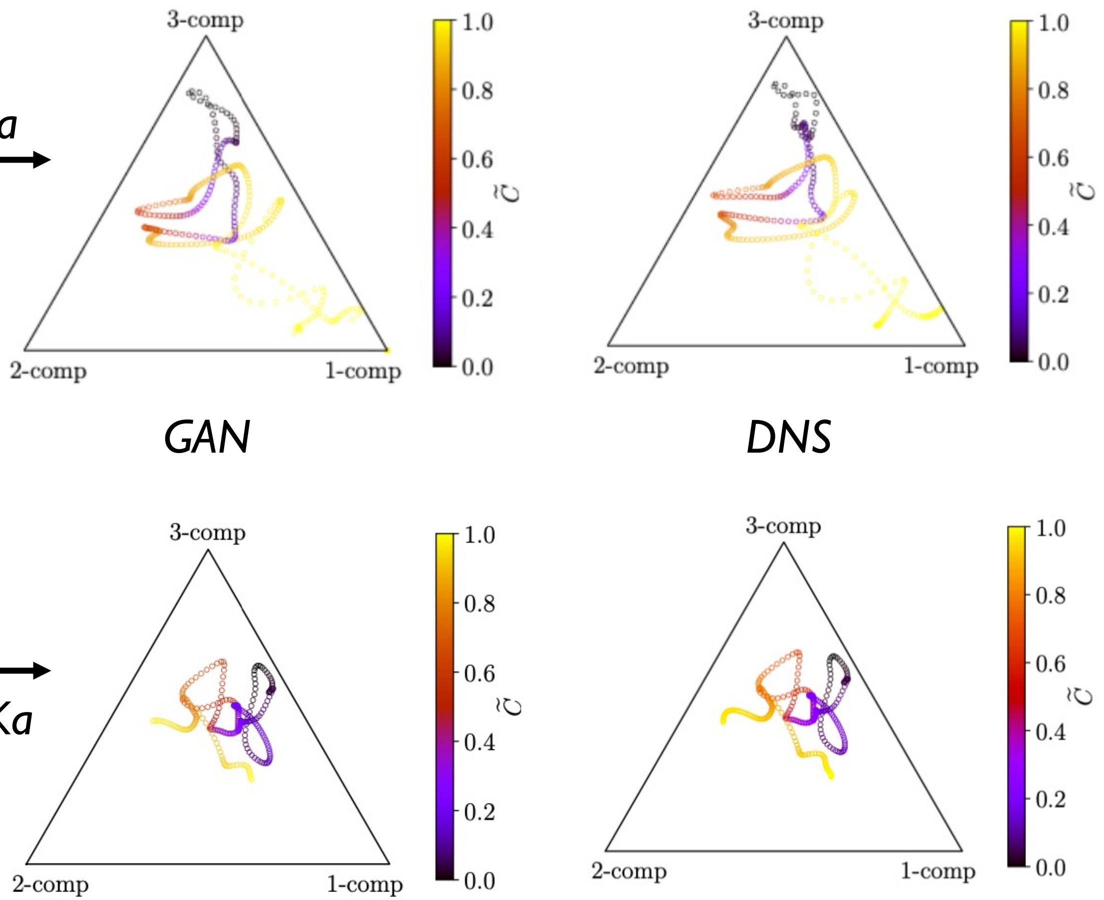
Premixed hydrogen/air flames DNS dataset

$Ka < Ka_{cr}$ (Low Ka)



$Ka > Ka_{cr}$ (High Ka)

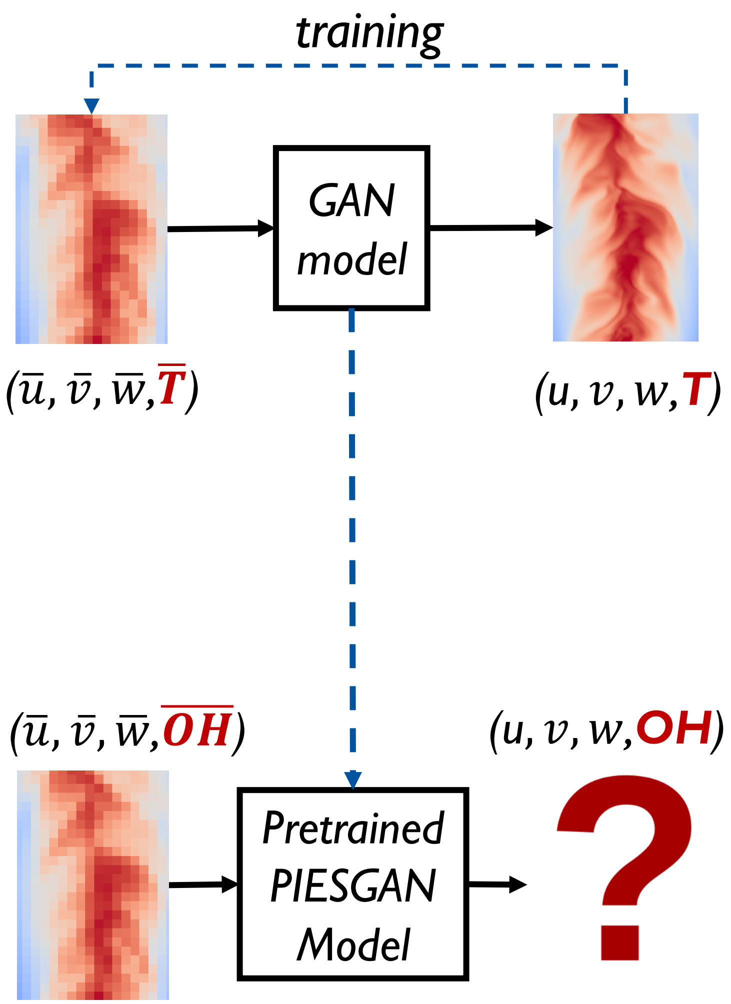
Barycentric maps of the Reynolds stress invariants

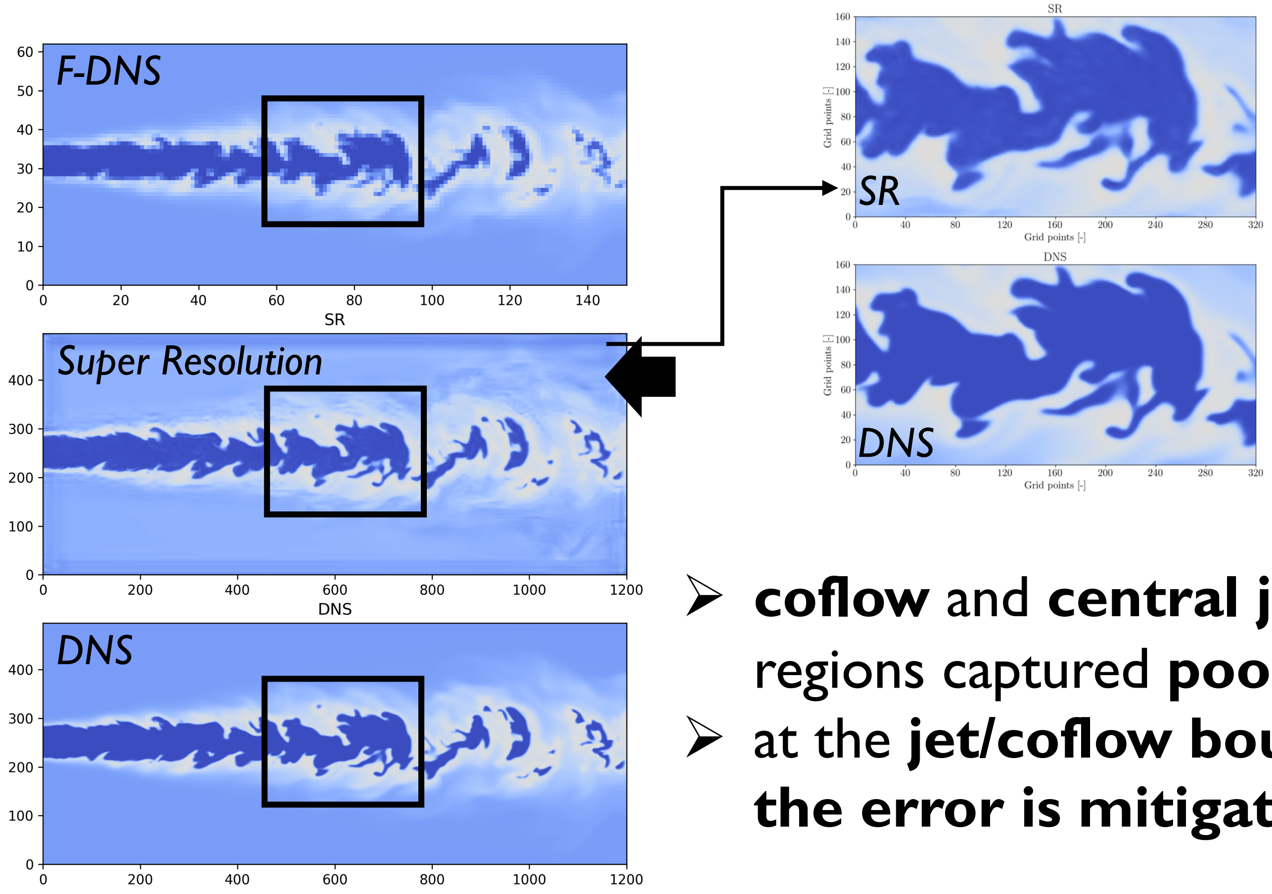


A shuffle training approach must be employed to achieve a **certain level of generalizability**

J. MacArt et al., “Effects of combustion heat release on velocity and scalar statistics in turbulent premixed jet flames”, Combustion and Flame, 2018
T. Grenga et al., “Predictive data-driven model based on generative adversarial network for premixed turbulence-combustion regimes”, CST, 2020

Generalization towards different physical quantities not included at the input





OH mass fraction

- **coflow** and **central jet** regions captured **poorly**
- at the **jet/coflow boundary, the error is mitigated**

L. Nista et al., "Investigation of the generalization capability of a GAN for LES of turbulent premixed reacting flows", Proc. Combust. Inst., 2022.

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Conclusion and future works

- PIESRGAN network performance is assessed **against a supervised** CNN-based network in the context of **turbulence closure modeling**
- a-priori in-sample analysis demonstrates the ability of the **GAN model to recover the DNS data**
  - a-priori **subfilter-scale GAN model outperforms** the dynamic Smagorinsky model
- a-priori **performance of far-from-training conditions** has been investigated
  - **the ratio Δ/η needs to be matched to ensure generalizability,** showing good extrapolation at both lower and higher Re
  - **Shuffle training approach** efficient to predict different combustion regimes

Future works

- perform additional investigations at different flow conditions
- further extrapolation and generalization capability
- a-posteriori embedding in a LES solver

Thank you for your attention

… and to the coauthors:

- **Mr. C. Schumann** – University of Cambridge, UK
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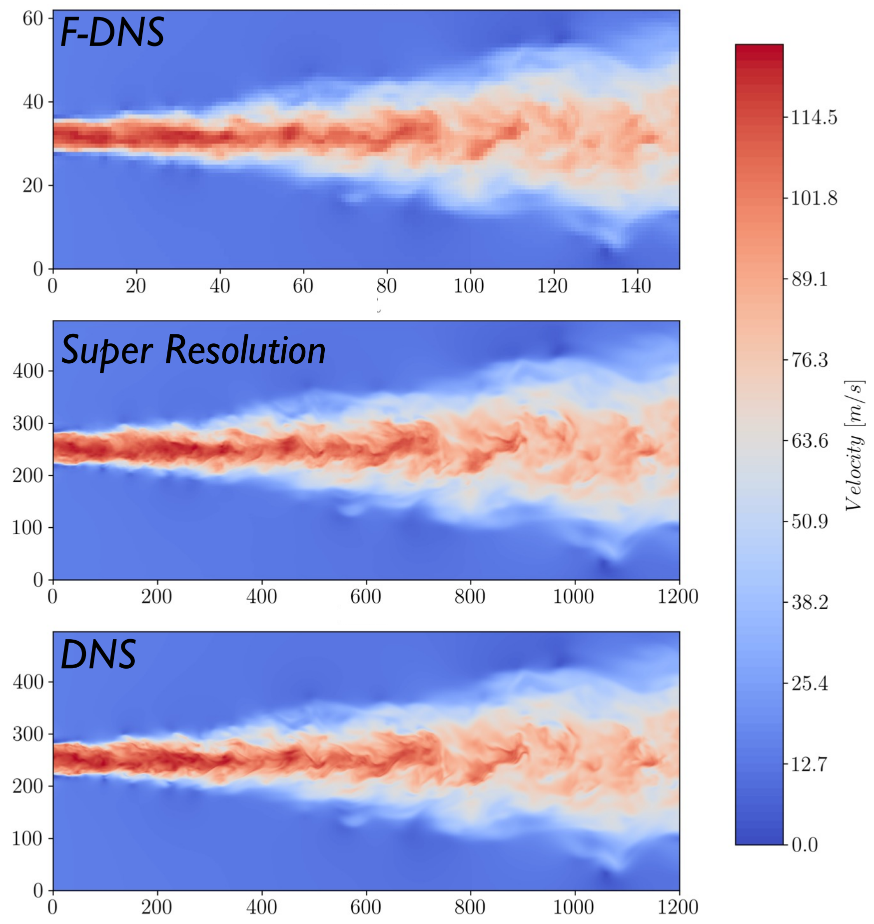

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