



Complex Fluids and Complex Flows Group
Dept. Physics & INFN - University of Rome 'Tor Vergata'

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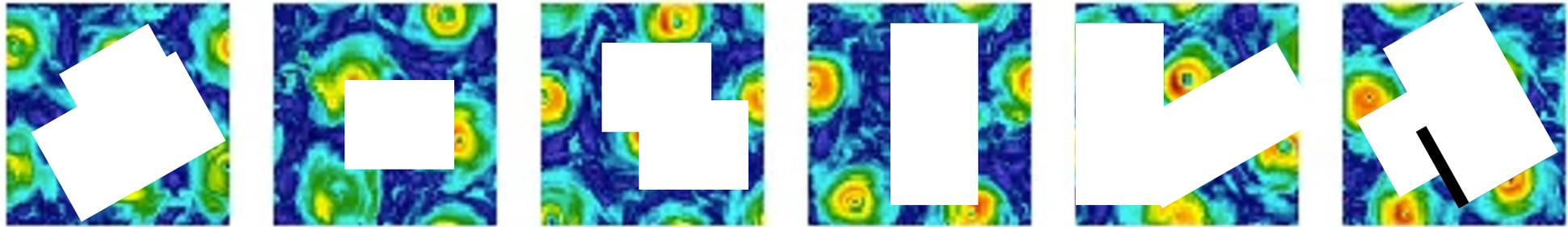
Damiano Capocci



Fabio Bonaccorso

CFDParSchool GSSI 2023

Equations-**Informed** and **Data**-Driven Tools For **Turbulent** Flows



Rotation rate?

Viscosity?

Reynolds number?

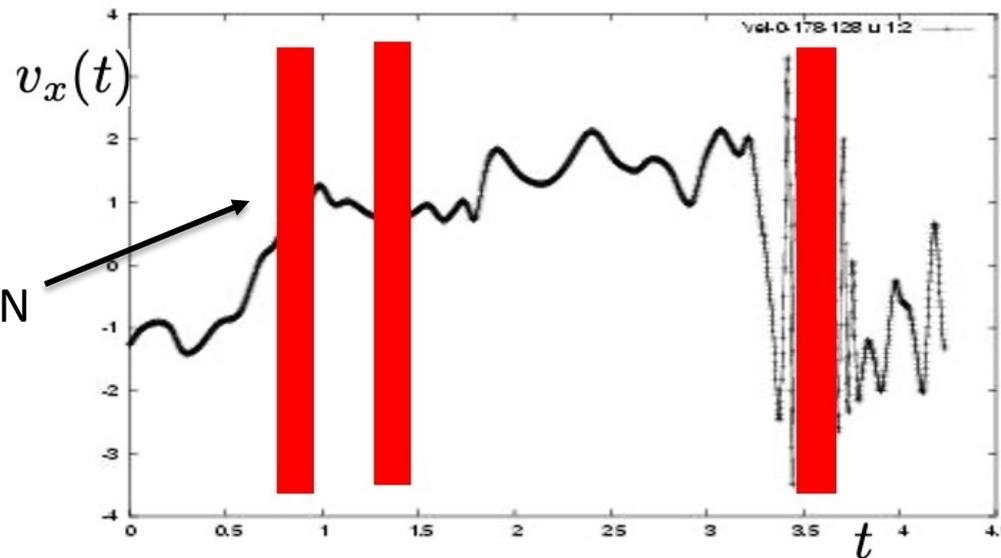
Boundary conditions?

Forcing properties?

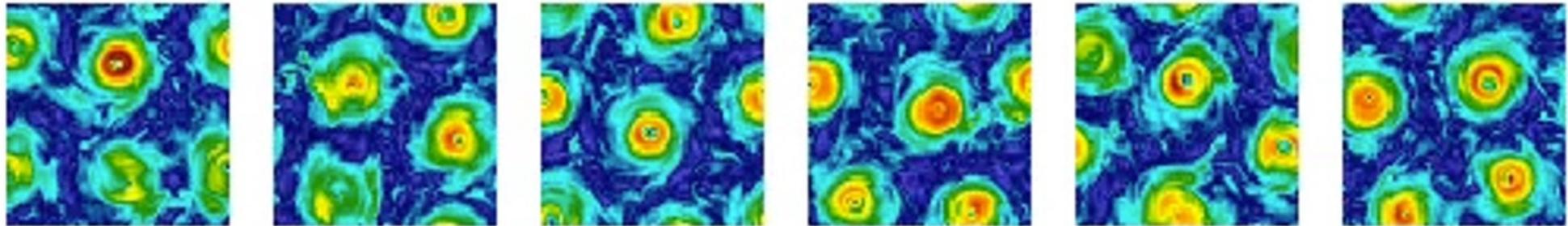
Aspect ratio?

EULERIAN

LAGRANGIAN



CREDITS: T. LI, M. BUZZICOTTI, S. CHEN. M. WAN



Rotation rate?

Viscosity?

Reynolds number?

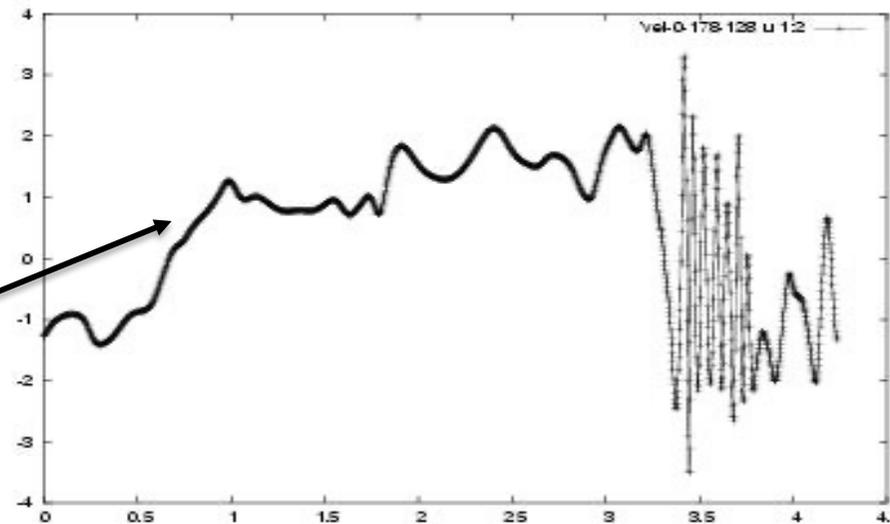
Boundary conditions?

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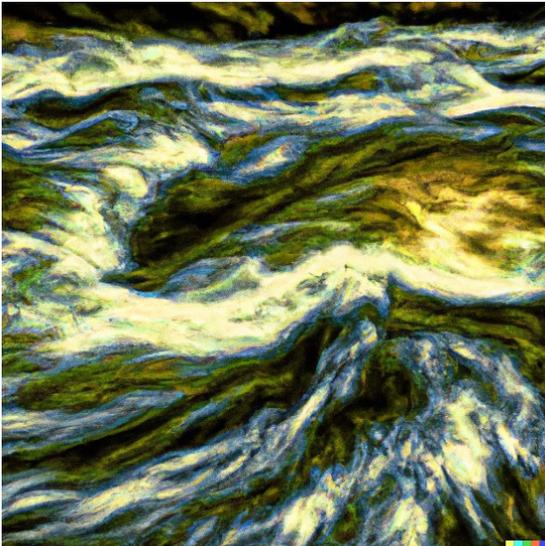
EULERIAN

LAGRANGIAN



1. Short introduction to Eulerian and Lagrangian Turbulence in 2D, 3D and in between
 2. Data-driven and Equation-Informed tools for Eulerian Turbulence
 3. Data-driven and Equation-Informed tools for Lagrangian Turbulence
-

A WATER COLOR STYLE IMAGE OF
A TURBULENT FLOW



MADE BY DALL-E OpenAI

A MIRO' STYLE IMAGE OF
A TURBULENT FLOW



MADE BY DALL-E OpenAI

A CUBIST STYLE IMAGE OF
A TURBULENT FLOW



MADE BY DALL-E OpenAI

COMPLEX FLUIDS & COMPLEX FLOWS

EULERIAN

$$\left\{ \begin{aligned} \partial_t v + v \cdot \partial_x v &= -\partial_x p + \nu \partial^2 v + g\theta + b \cdot \partial_x b + f + \sum_i \delta(x - X_i) \mathcal{F} \\ \partial_x \cdot v &= 0 \\ +b.c. \end{aligned} \right.$$

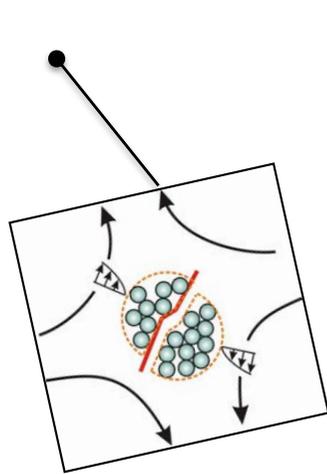
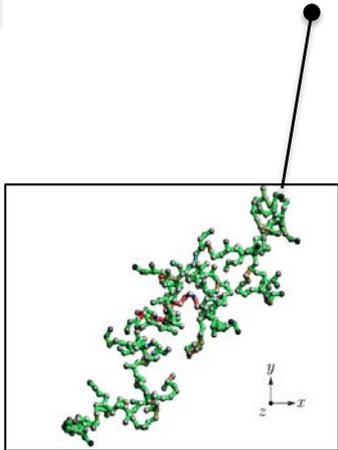
temperature

magnetic field

small active/passive particles/droplets/bubbles/colloidal aggregates

LAGRANGIAN

$$\left\{ \begin{aligned} \dot{X}_i &= U_i \\ \dot{U}_i &= \frac{v(X_i) - U_i}{\tau} + \beta D_t v(X_i) + U_i^C \end{aligned} \right.$$



COMPLEX FLUIDS & COMPLEX FLOWS

EULERIAN

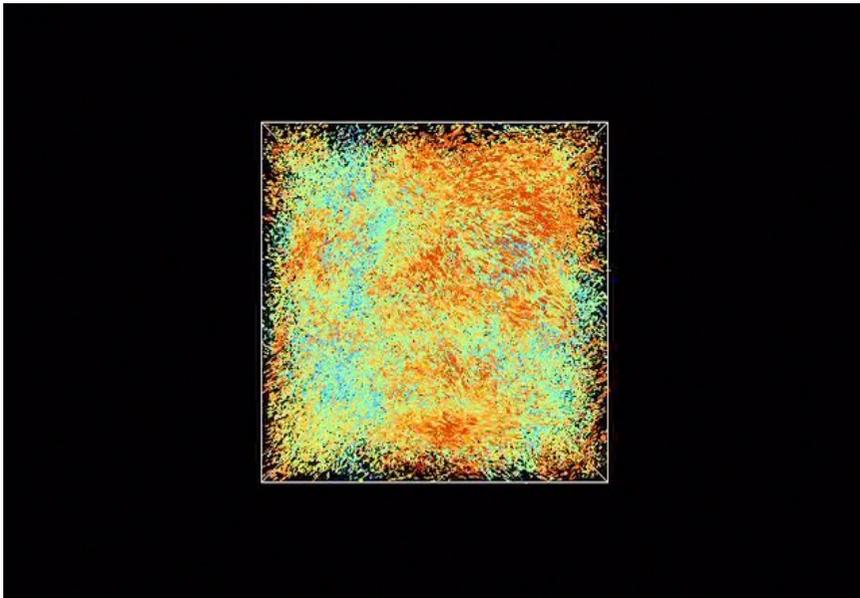
$$\left\{ \begin{array}{l} \partial_t v + v \cdot \partial_x v = -\partial_x p + \nu \partial^2 v \quad \text{[grey box]} + f \quad \text{[grey box]} \\ \partial_x \cdot v = 0 \\ +b.c. \end{array} \right.$$

temperature

magnetic field

LAGRANGIAN

$$\left\{ \dot{X}_i = v(X_i(t), t) \right. \leftarrow \text{passive fluid tracers}$$



CONTROL PARAMETER:

$$Re \sim \frac{v \partial_x v}{\nu \partial^2 v} \sim \frac{v_0 L_0}{\nu}$$

NAVIER-STOKES 3D-2D:
DIMENSIONS MATTER!

2D

Entry #: 84174

3D

Vortices within vortices: hierarchical nature of vortex tubes in turbulence

Kai Bürger¹, Marc Treib¹, Rüdiger Westermann¹,
Suzanne Werner², Cristian C Lalescu³,
Alexander Szalay², Charles Meneveau⁴, Gregory L Eyink^{2,3,4}

¹ Informatik 15 (Computer Graphik & Visualisierung), Technische Universität München

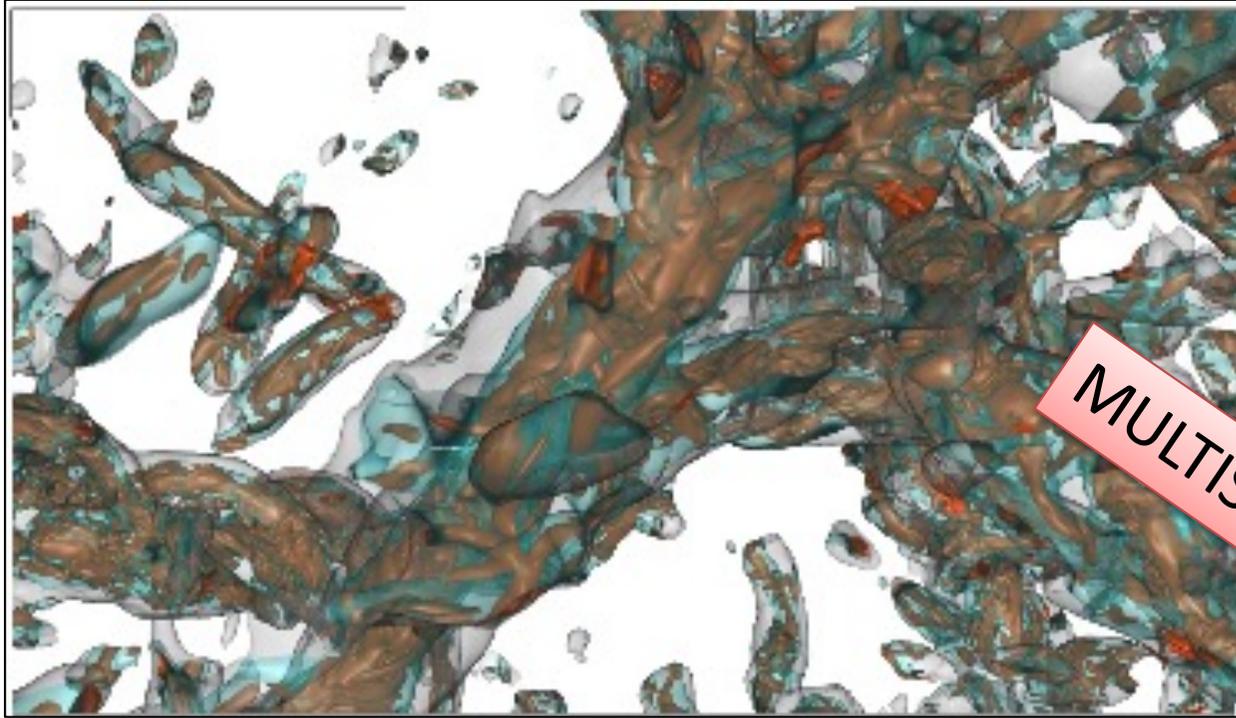
² Department of Physics & Astronomy, The Johns Hopkins University

³ Department of Applied Mathematics & Statistics, The Johns Hopkins University

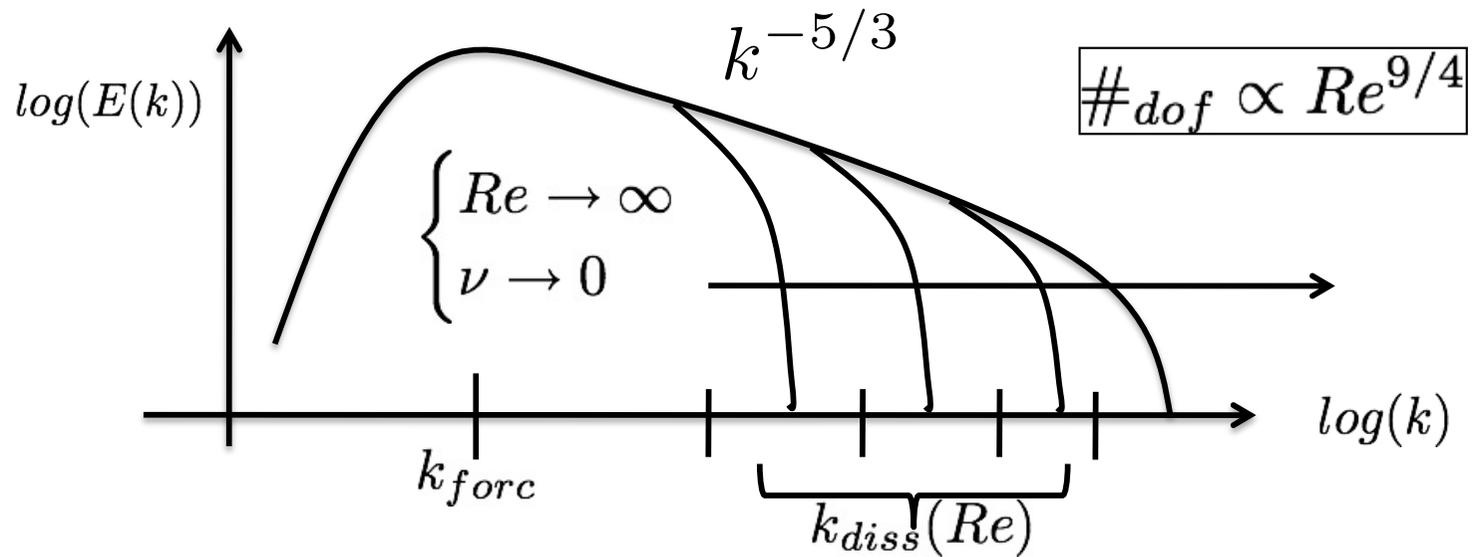
⁴ Department of Mechanical Engineering, The Johns Hopkins University

ULTRAVIOLET (3D)
AND INFRARED (2D)
PHYSICS

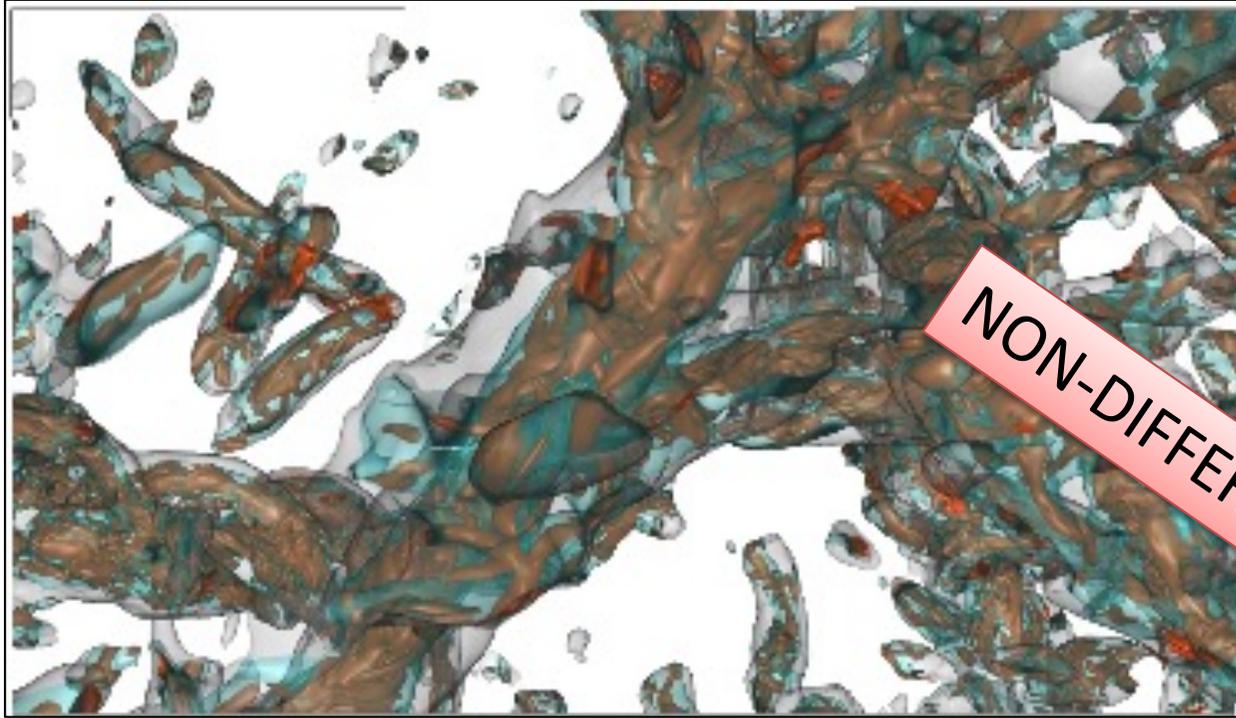
NAVIER-STOKES 3D



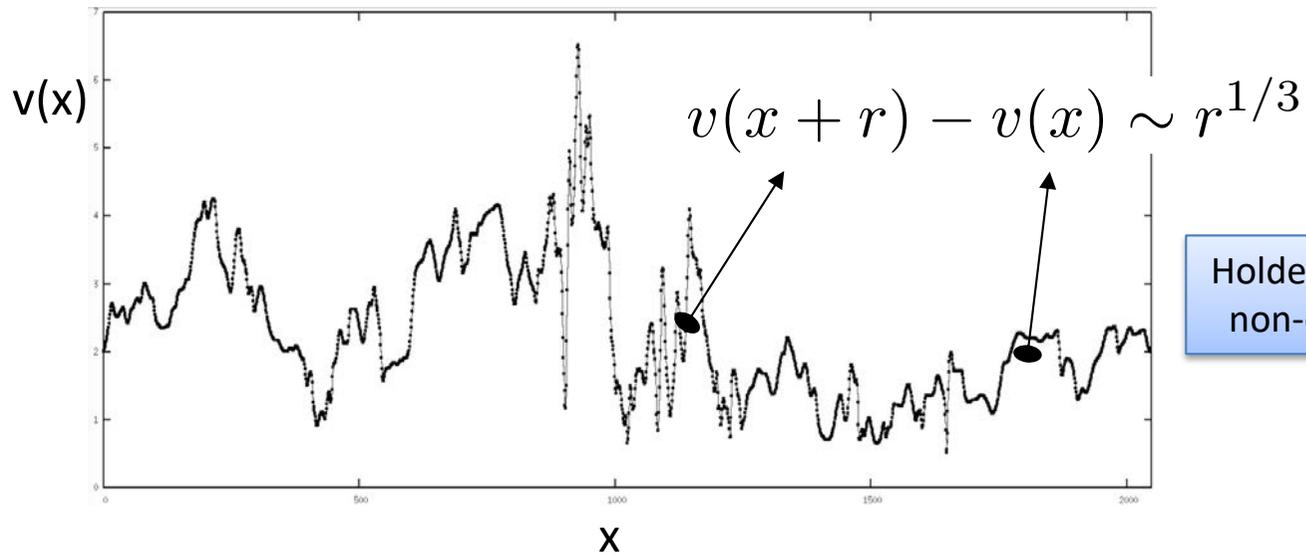
MULTISCALE!



NAVIER-STOKES 3D

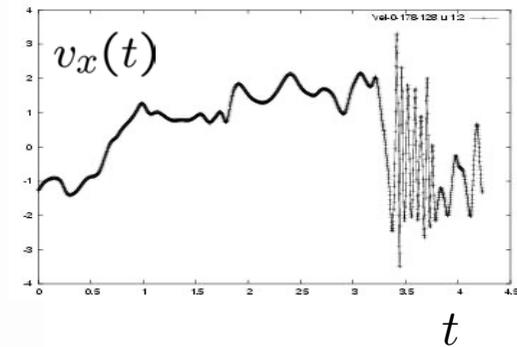
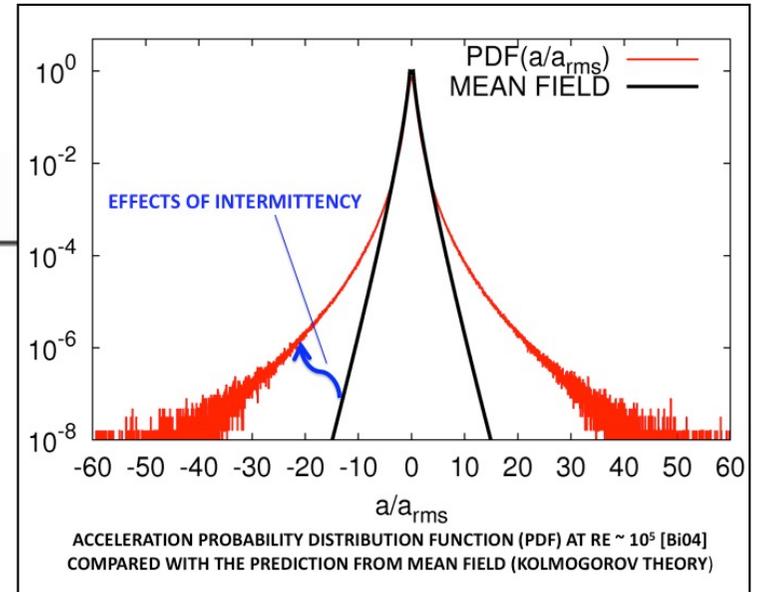
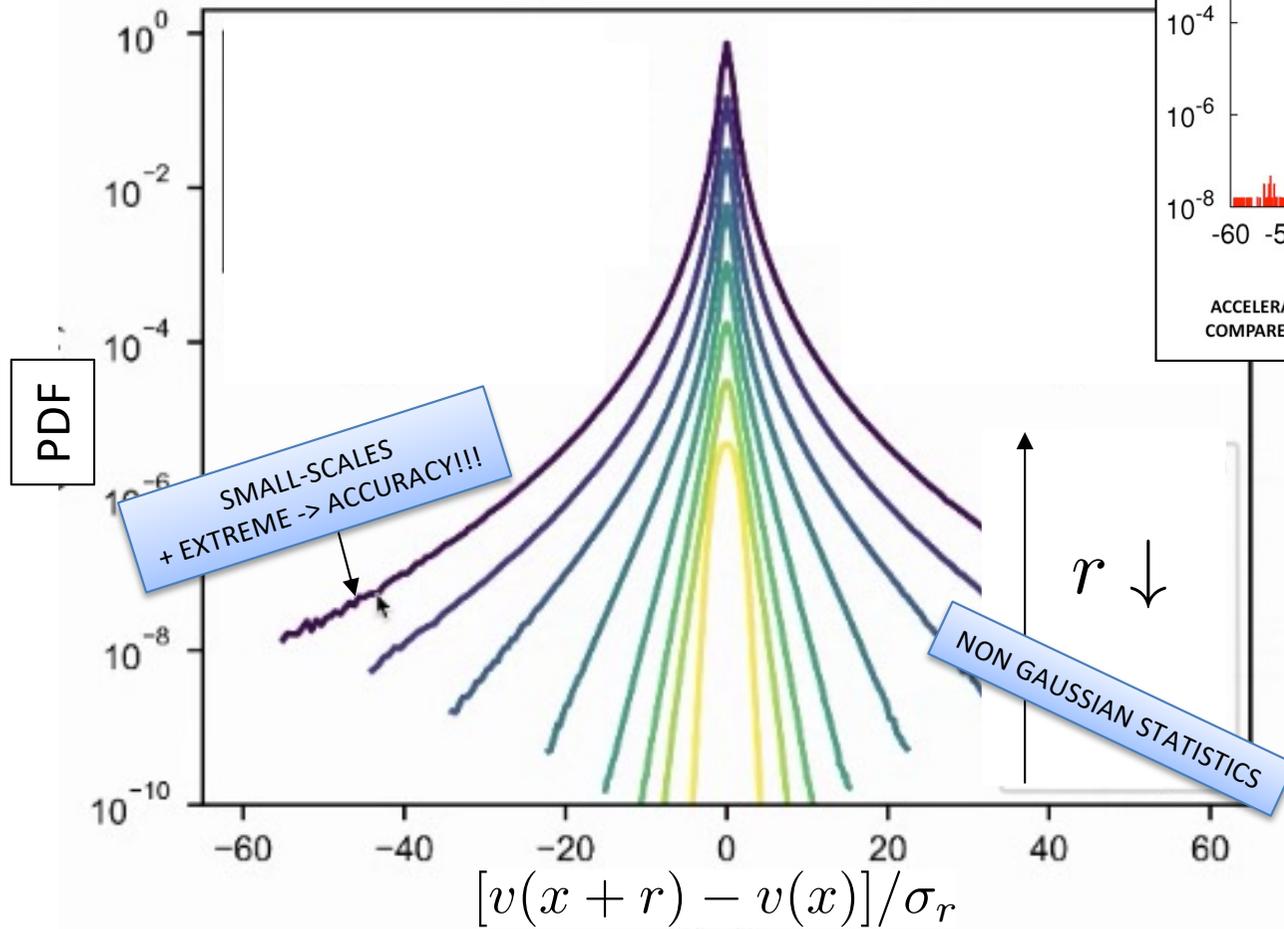


NON-DIFFERENTIABLE !



Holder continuous 1/3
non-differentiable!

NAVIER-STOKES 3D



Bentkamp, L, Cr C. Lalescu, and M. Wilczek. "Nature communications 10.1 (2019): 1-8.

COMPLEX FLUIDS & COMPLEX FLOWS

EULERIAN

$$\left\{ \begin{aligned} \partial_t v + v \cdot \partial_x v &= -\partial_x p + \nu \partial^2 v + g\theta + b \cdot \partial_x b + f + \sum_i \delta(x - X_i) \mathcal{F} \\ \partial_x \cdot v &= 0 \\ +b.c. \\ \partial_t \theta + v \cdot \partial_x \theta &= \chi_\theta \partial^2 \theta \\ \partial_t b + v \cdot \partial_x b - b \cdot \partial_x v &= \chi_b \partial^2 b \end{aligned} \right.$$

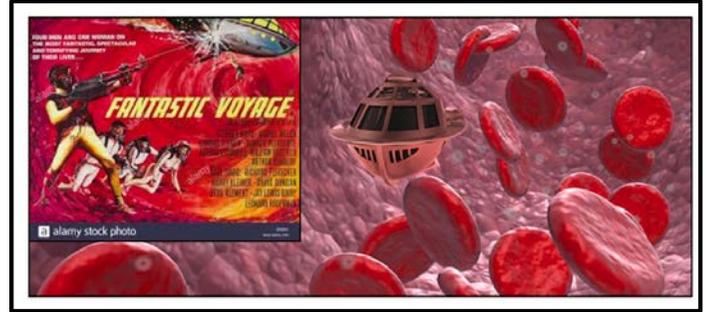
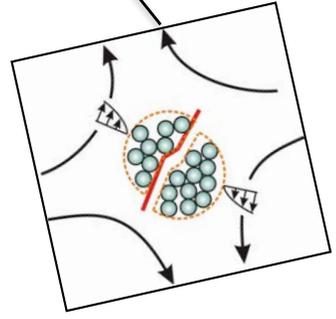
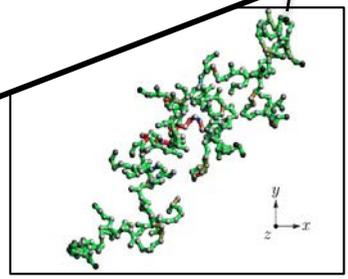
temperature

LAGRANGIAN

$$\left\{ \begin{aligned} \dot{X}_i &= U_i \\ \dot{U}_i &= \frac{v(X_i) - U_i}{\tau} \end{aligned} \right.$$

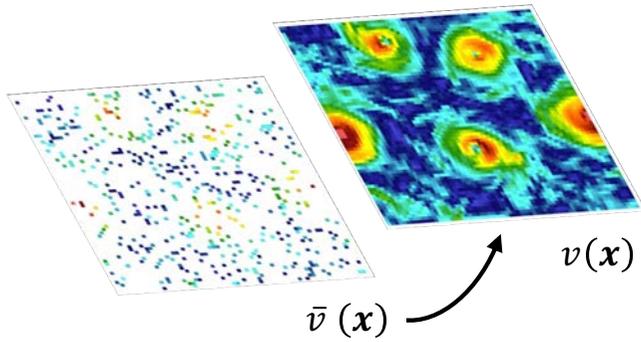
droplets/bubbles/colloidal aggregates

1. NO WAY TO PREDICT STATISTICS FOR MEAN PROFILES OR EXTREME EVENTS FROM EOM
 2. NO WAY TO PERFORM DIRECT NUMERICAL SIMULATIONS FOR REALISTIC PROBLEMS
WE NEED QUANTITATIVE MODELS AND TOOLS TO MODEL!

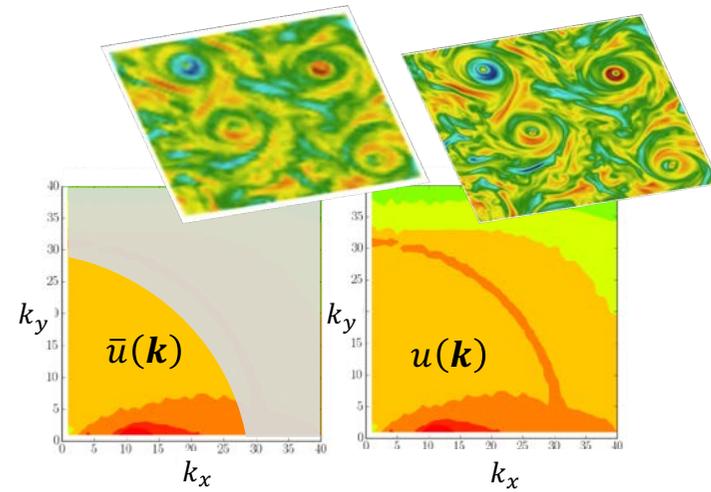


(BIG) DATA ASSIMILATION

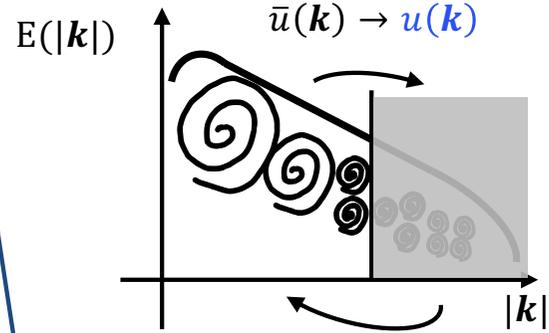
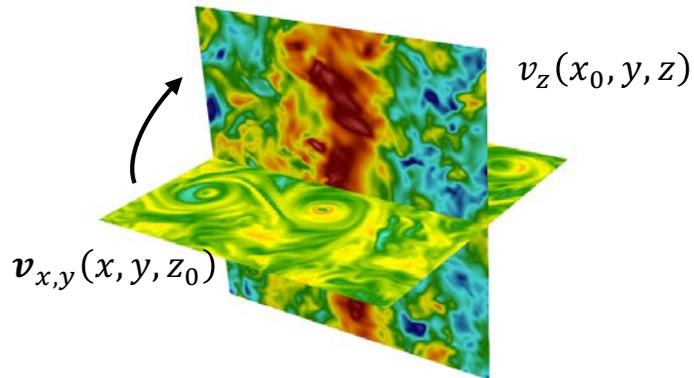
(i) Real-space Reconstruction (full state)



(iii) Fourier-space Reconstruction (Super Resolution)

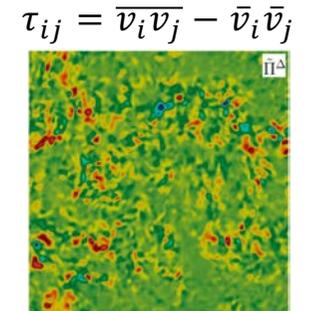


(ii) Missing Physics (Inverse Problems)



(iv) Sub-Grid Modeling

$$\bar{u}(\mathbf{k}) \rightarrow \partial_t \bar{u}(\mathbf{k}) = \dots + \nabla \cdot \tau$$

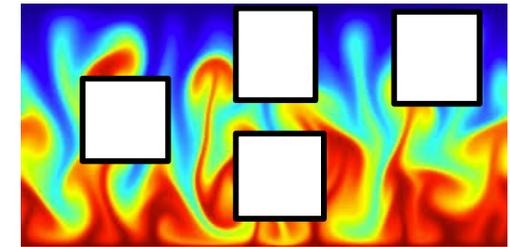
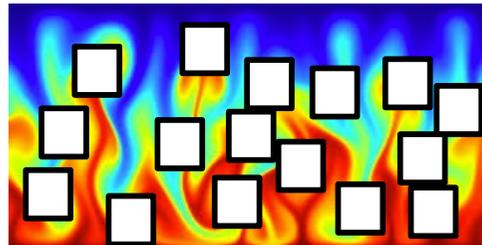
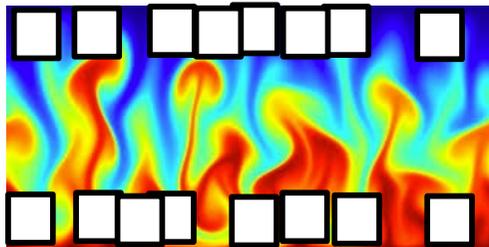


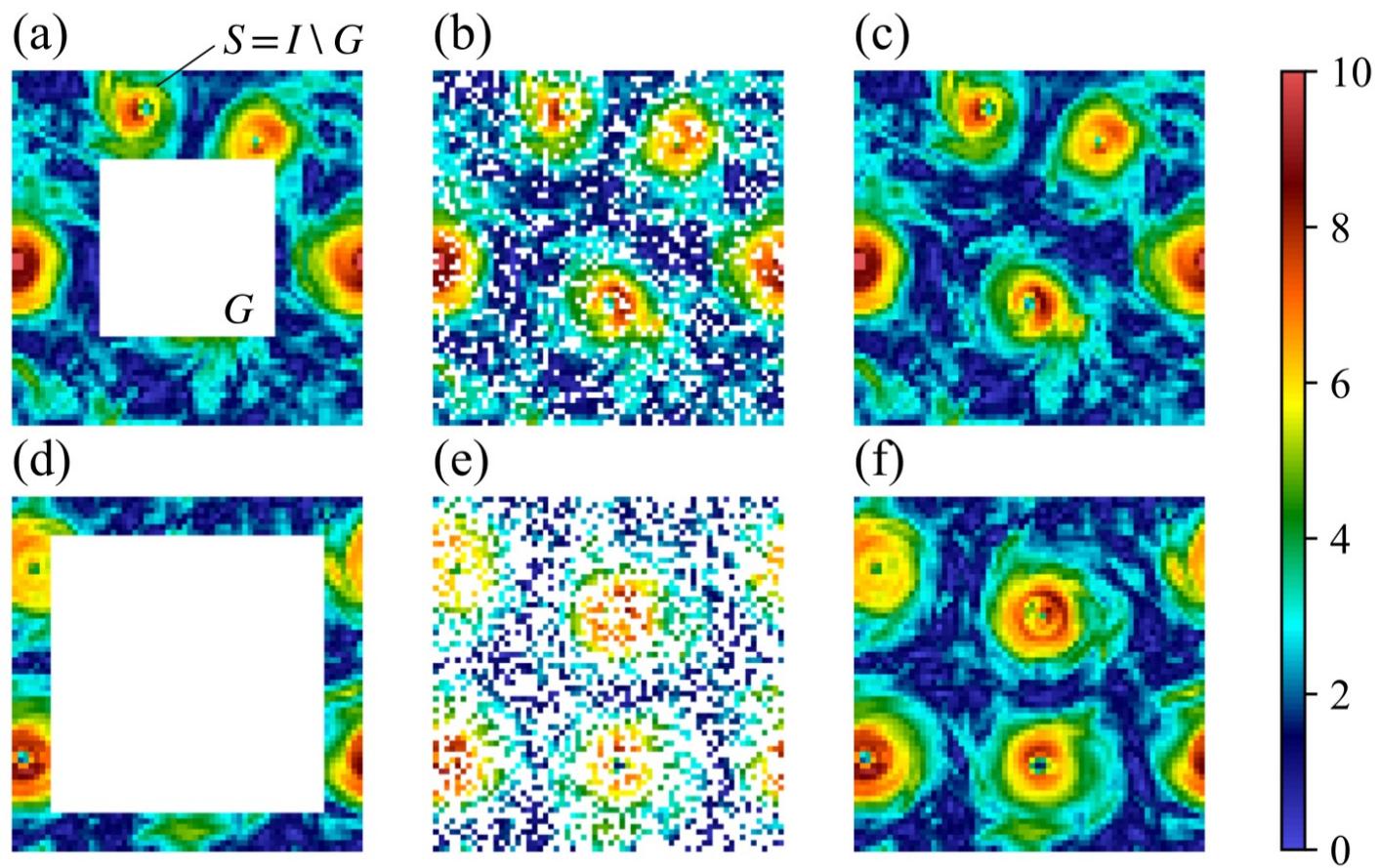
1. RECONSTRUCTION OF MISSING INFORMATION (INPAINTING – SUPER RESOLUTION)

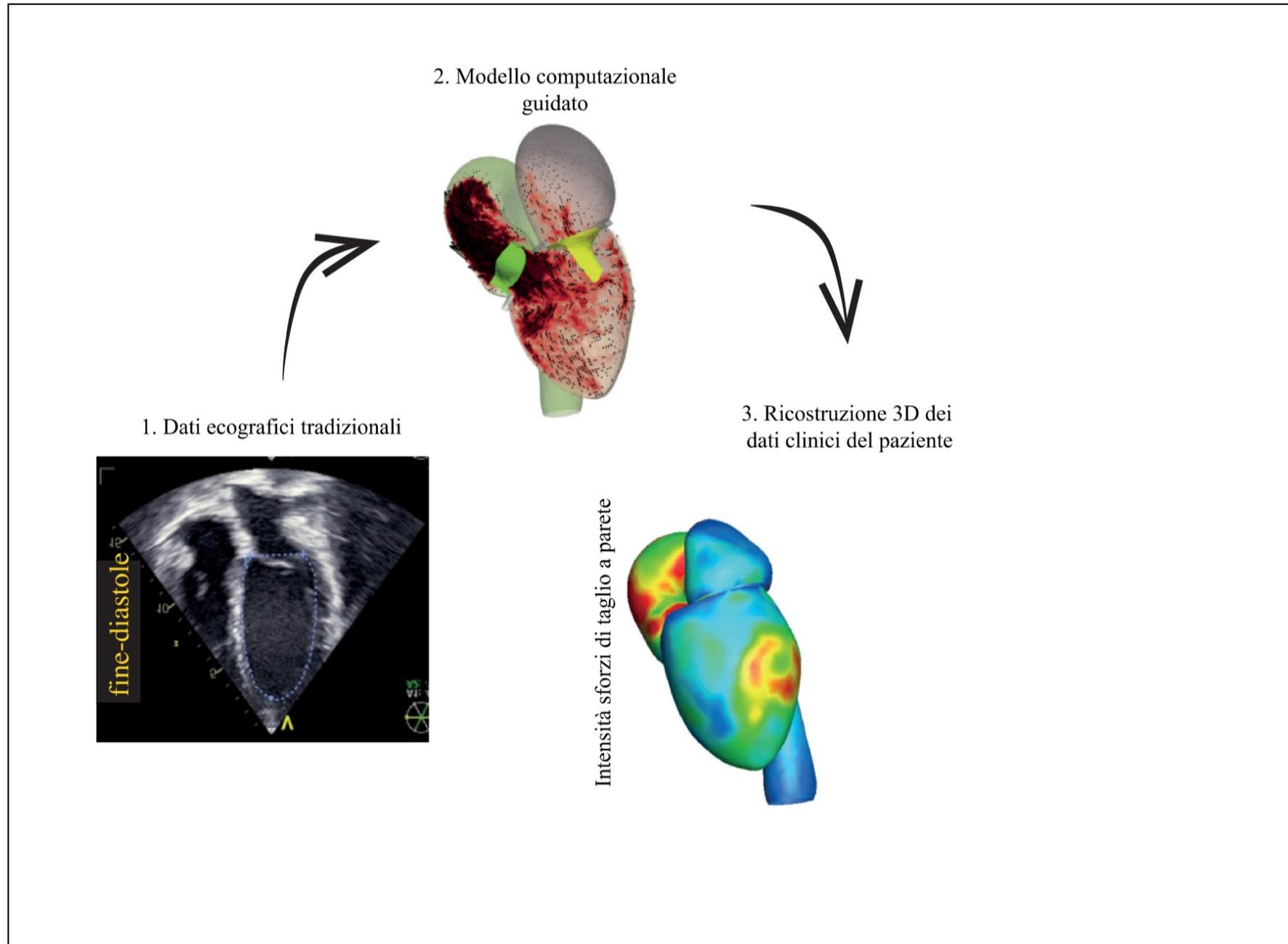
2. FEATURES RANKING: QUALITY AND QUANTITY OF DATA

- IS IT BETTER TO INPUT SPATIAL OR TEMPORAL DATA?
- HOW MANY DATA/VARIABLES YOU NEED TO SUPPLY FOR PERFECT RECONSTRUCTION (SYNCHRONIZATION-TO-DATA)?
- CAN YOU GUESS VELOCITY FIELDS BY MEASURING ONLY TEMPERATURE AND/OR VICEVERSA?
- IS IT BETTER TO PROVIDE INFORMATION FROM BOUNDARIES OR BULK?
- FROM LARGE OR SMALL SCALES?
- DO WE NEED TO KNOW THE EQUATIONS?
- HOW TO COMPARE EQUATIONS-BASED AND EQUATIONS-FREE MODELS?

A WAY TO LEARN ABOUT THE UNDERLYING PHYSICS

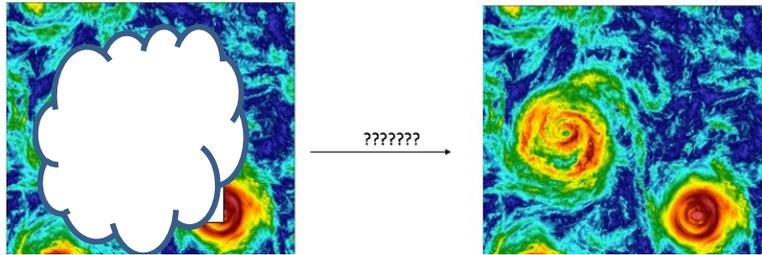






with F. Viola (GSSI) and R. Verzicco (U Tor Vergata)

DATA ASSIMILATION, FLOW RECONSTRUCTION, INPAINTING, SUPER-RESOLUTION, PHYSICS-INFERRING (CLASSIFICATION)

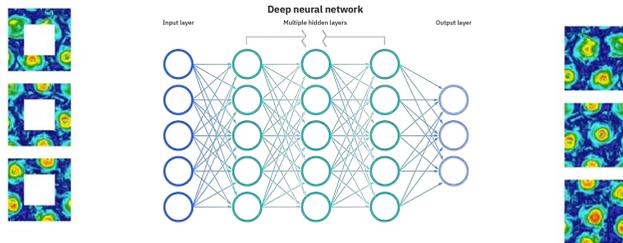


DATA
DRIVEN

$$u(\mathbf{x}) = \sum_{n=1}^N a_n \psi_n(\mathbf{x}) = \sum_{n=1}^{N'} a_n \psi_n(\mathbf{x}) + \sum_{n=N'+1}^N a_n \psi_n(\mathbf{x})$$

$$\int_S \left[u(\mathbf{x}) - \sum_{n=1}^{N'} a_n \psi_n(\mathbf{x}) \right]^2 dx$$

1. EQUATION FREE
PRINCIPAL ORTHOGONAL DECOMPOSITION
GAPPY-POD & EXTENDED POD



2. EQUATION FREE
GENERATIVE-ADVERSARIAL-NETWORK

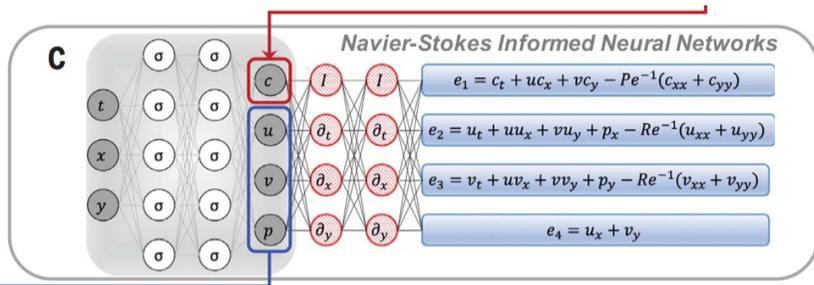
EQ.
BASED

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} + 2\Omega \hat{x}_3 \times \mathbf{v} = -\nabla p + \nu \nabla^2 \mathbf{v} + \gamma(1 - \hat{M})_{x_3} \odot (\mathbf{v} - \mathbf{v}_{\text{ref}})$$

3. NUDGING

DATA
DRIVEN

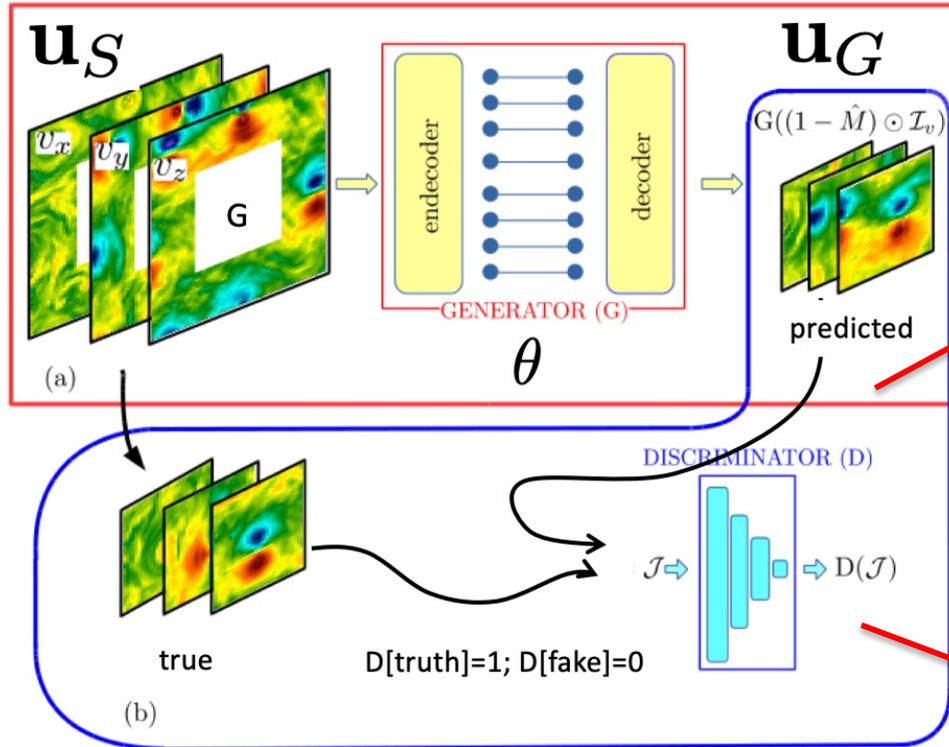
EQ.
BASED



$$MSE = \frac{1}{N} \sum_{n=1}^N \left| c(t^n, \mathbf{x}^n, \mathbf{y}^n, \mathbf{z}^n) - \hat{c}^n \right|^2 + \sum_{i=1}^5 \frac{1}{M} \sum_{m=1}^M \left| e_i(t^m, \mathbf{x}^m, \mathbf{y}^m, \mathbf{z}^m) \right|^2$$

4. PINN
Physics-Informed NN

GENERATIVE ADVERSARIAL NETWORK: CONTEXT ENCODER (ACTOR-CRITIC)



MINIMIZE:

$$\mathcal{L}_{GEN} = (1 - \lambda_{adv})\mathcal{L}_{MSE} + \lambda_{adv}\mathcal{L}_{adv},$$

$$\mathcal{L}_{MSE} = \left\langle \frac{1}{A(I)} \int_I \|\mathbf{u}_G^{(p)}(\mathbf{x}) - \mathbf{u}_G^{(t)}(\mathbf{x})\|^2 d\mathbf{x} \right\rangle$$

$$\mathcal{L}_{adv} = \langle \log(1 - D(\mathbf{u}_G^{(p)})) \rangle$$

$$= \int p(\mathbf{u}_S) \log[1 - D(GEN(\mathbf{u}_S))] d\mathbf{u}_S$$

MAXIMIZE:

$$\mathcal{L}_{DIS} = \langle \log(D(\mathbf{u}_G^{(t)})) \rangle + \langle \log(1 - D(\mathbf{u}_G^{(p)})) \rangle$$

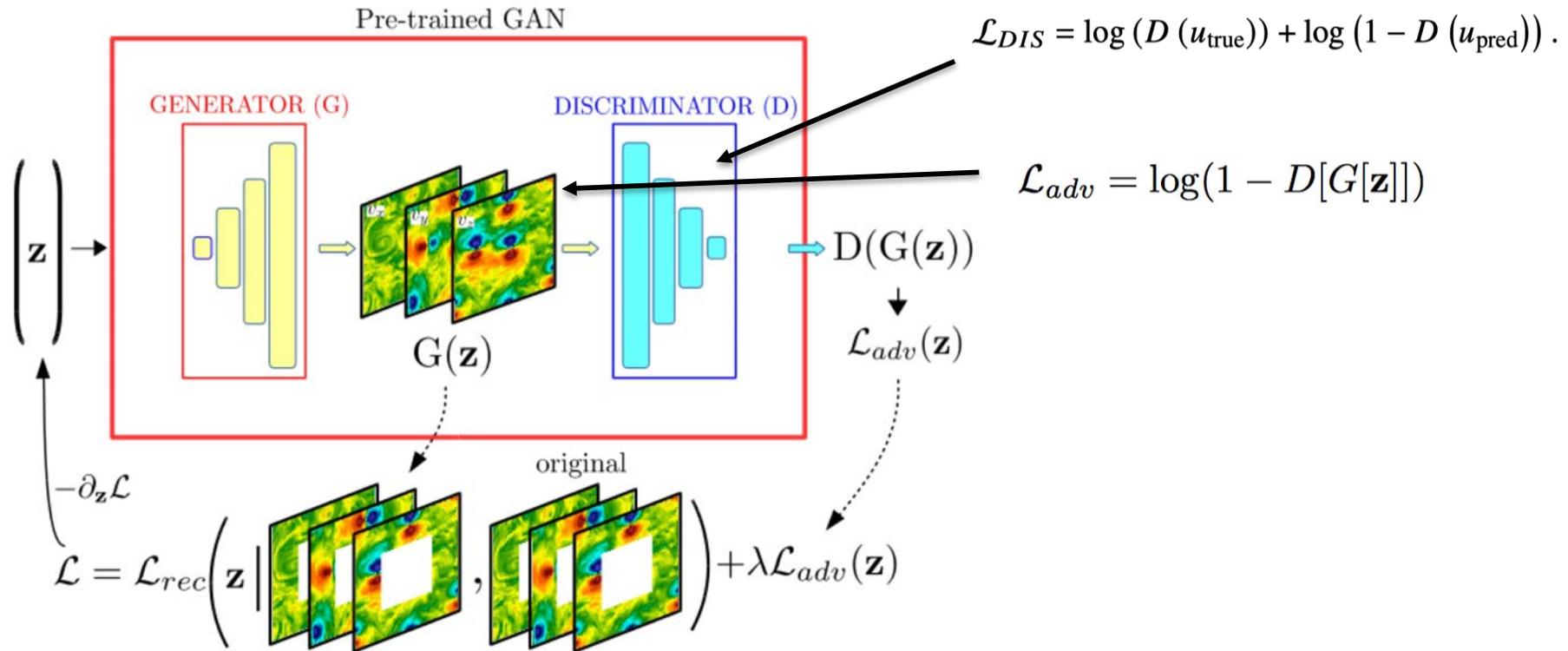
$$= \int [p_t(\mathbf{u}_G) \log(D(\mathbf{u}_G)) +$$

$$p_p(\mathbf{u}_G) \log(1 - D(\mathbf{u}_G))] d\mathbf{u}_G.$$

$$D^*(\mathbf{u}) = \frac{p_t(\mathbf{u})}{p_t(\mathbf{u}) + p_p(\mathbf{u})}$$

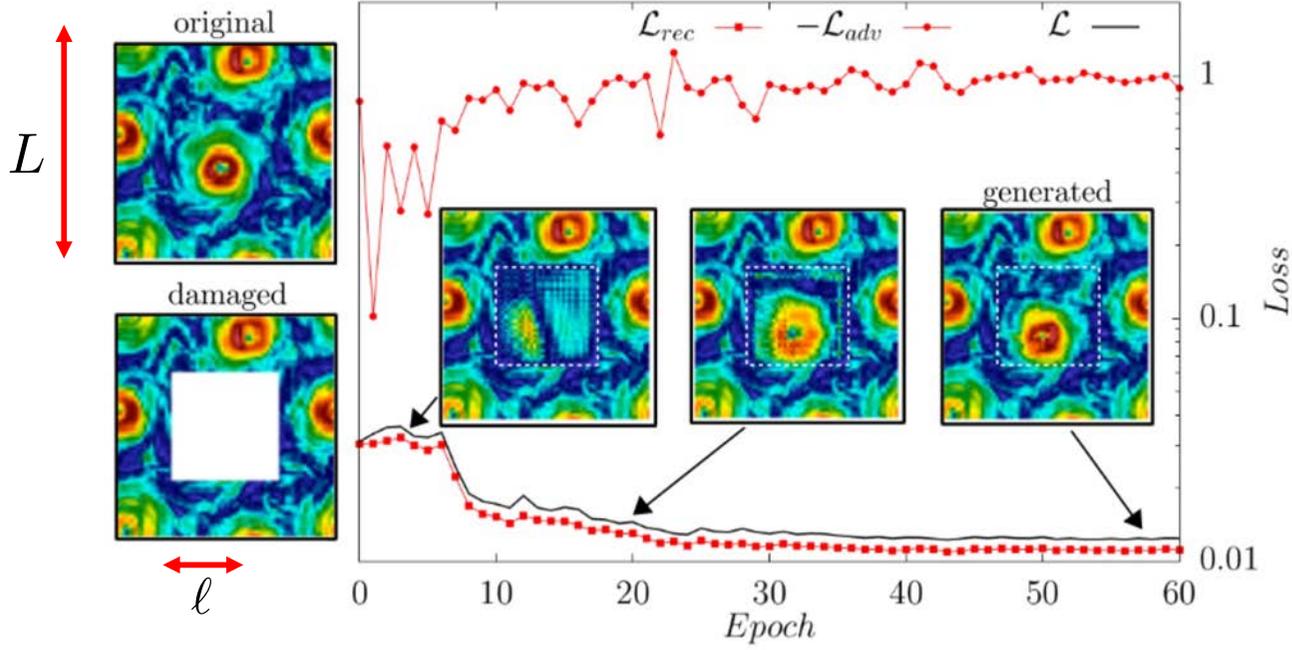
$$KL(p_t \parallel p_p) = \int_{-\infty}^{\infty} p_t(x) \log \left(\frac{p_t(x)}{p_p(x)} \right) dx$$

CONTEXT ENCODER 2 (CE2)
CONSTRAINED IMAGE GENERATION



Raymond A Yeh, Chen Chen, Teck Yian Lim, Alexander G Schwing, Mark Hasegawa-Johnson, and Minh N Do. Semantic image inpainting with deep generative models. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 5485–5493, 2017.

DURING TRAINING
80K 64x64 images of velocity amplitude for training
20K 64x64 images of velocity amplitude for validation



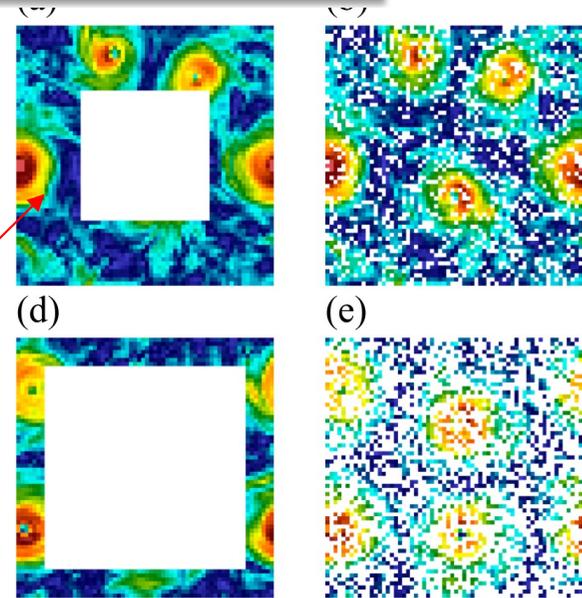
l :much larger than differentiable scale, i.e. velocity fields are rough (no linear interpolation here)

GAPPY-POD (PRINCIPAL ORTHOGONAL DECOMPOSITION)

$$u_{pred}(\mathbf{x}) = \sum_{n=1}^N a_n \psi_n(\mathbf{x}) = \sum_{n=1}^{N'} a_n \psi_n(\mathbf{x}) + \sum_{n=N'+1}^N a_n \psi_n(\mathbf{x}),$$

$$K(\mathbf{x}, \mathbf{y}) = \langle u_{true}(\mathbf{x}) u_{true}(\mathbf{y}) \rangle$$

$$\int K(\mathbf{x}, \mathbf{y}) \psi_n(\mathbf{y}) d\mathbf{y} = \lambda_n \psi_n(\mathbf{x})$$



$$X' = \psi \oplus \psi$$

$$\tilde{E} = \left\| \tilde{\mathbf{u}} - \tilde{X}' \mathbf{a}' \right\| = \int_S d\mathbf{x} \left(u_{true}(\mathbf{x}) - \sum_{n=1}^{N'} a_n \psi_n(\mathbf{x}) \right)^2$$

LINEAR OPTIMAL
REGRESSION

T. Li, L. Buzzicotti, F. Bonaccorso, L.B., S. Chen, M. Wan. Data reconstruction of turbulent flows with Gappy-POD and Generative Adversarial Networks. Submitted to JFM 2022.

EXTENDED-POD (PRINCIPAL ORTHOGONAL DECOMPOSITION)

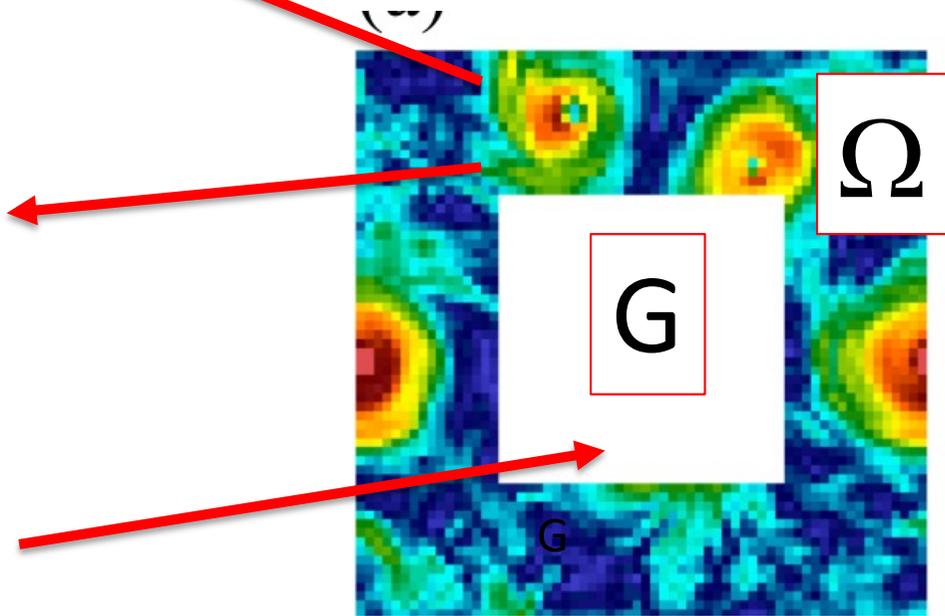
$$\int_{\Omega} R_S(x, y) \phi_S^{(n)}(y) dy = \sigma_n \phi_S^{(n)}(x),$$

$$u_S(x) = \sum_{n=1}^{N_S} b_S^{(n)} \phi_S^{(n)}(x),$$

$$\phi_S^{(n)}(x) = \langle b_S^{(n)} u_S(x) \rangle / \sigma_n.$$

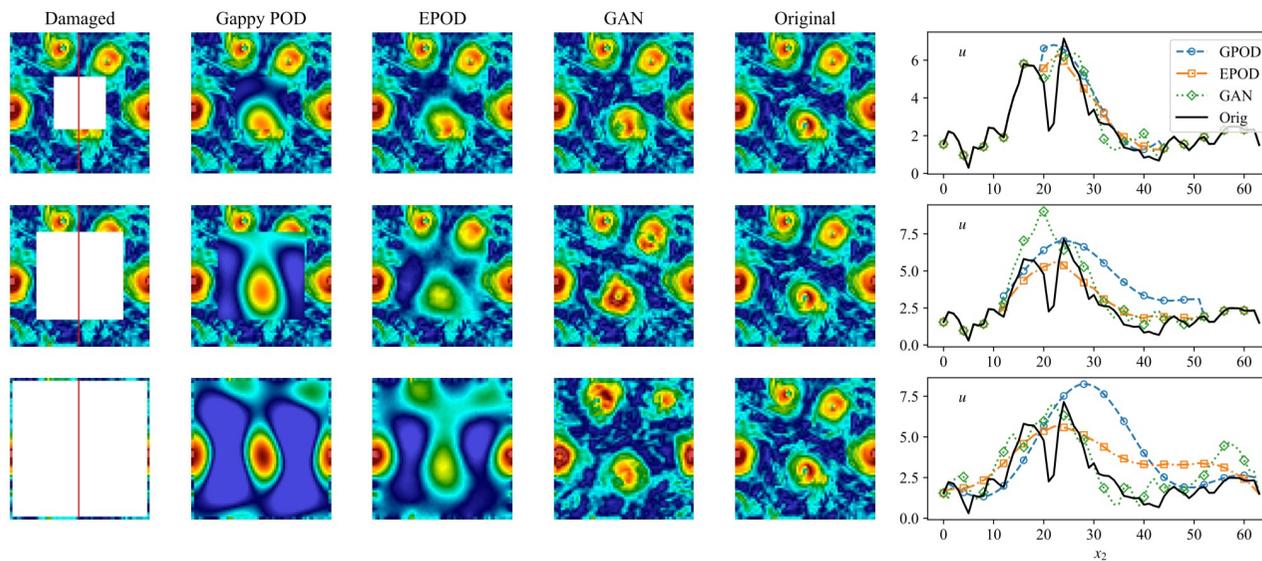
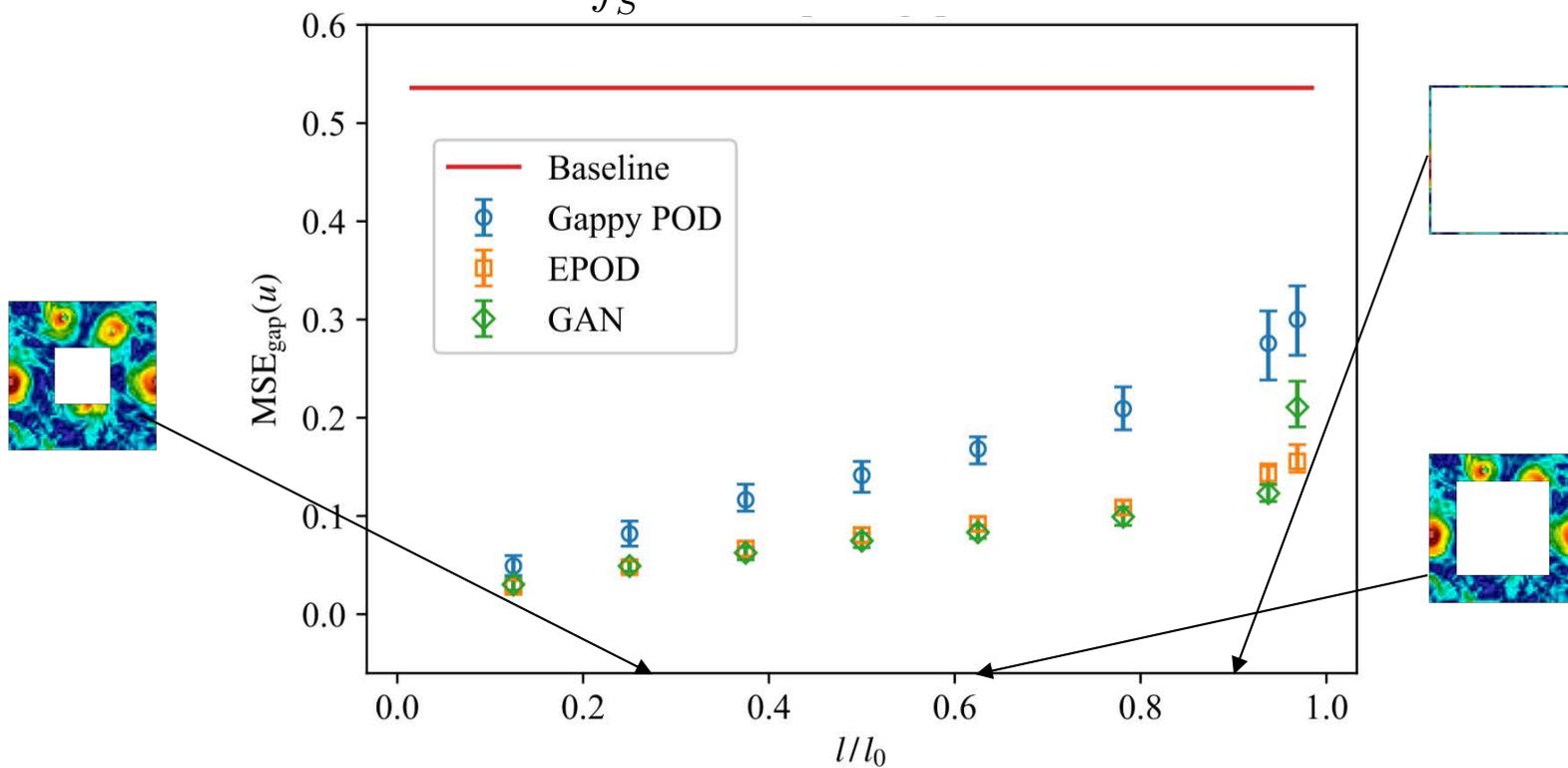


$$\phi_E^{(n)}(x) = \langle b_S^{(n)} u_G(x) \rangle / \sigma_n.$$

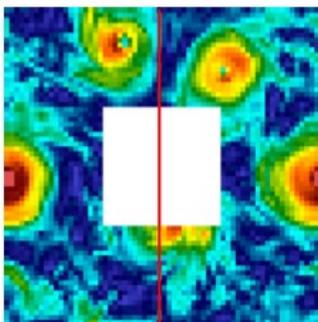


$$u_G^{(p)}(x) = \sum_{n=1}^{N_S} b_S^{(n)} \phi_E^{(n)}(x).$$

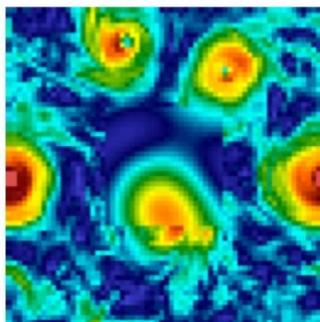
$$\mathcal{L}_G = \left\langle \int_S d\mathbf{x} (u_{true}(\mathbf{x}) - u_{pred}(\mathbf{x}, \theta))^2 \right\rangle$$



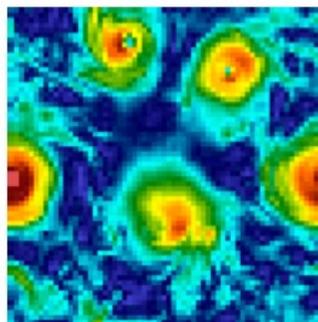
Damaged



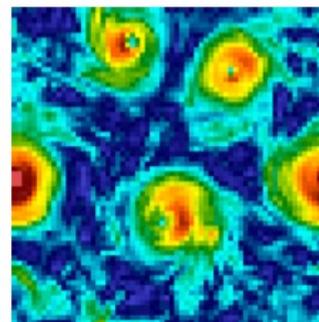
Gappy POD



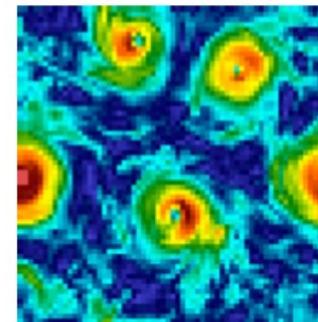
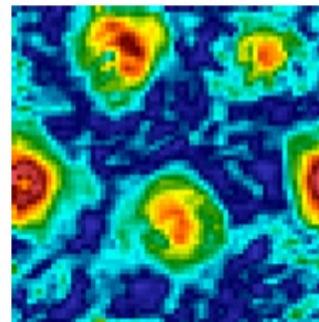
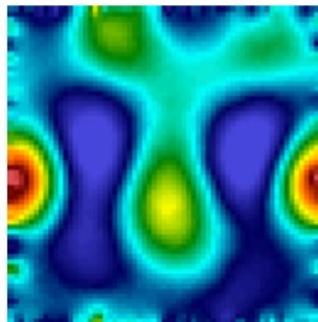
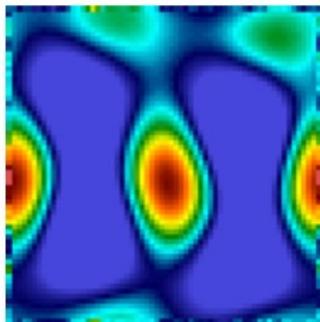
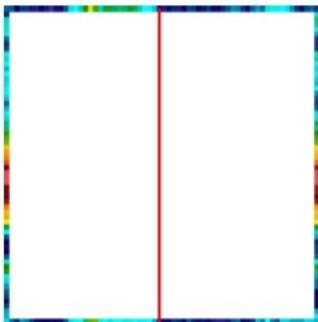
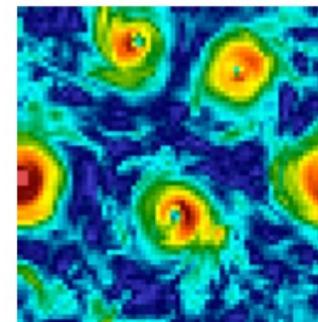
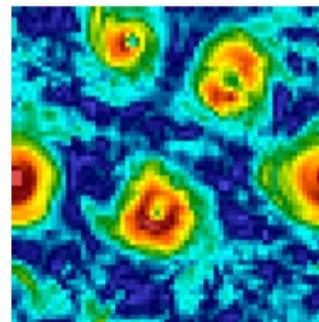
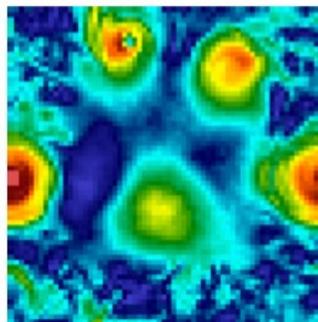
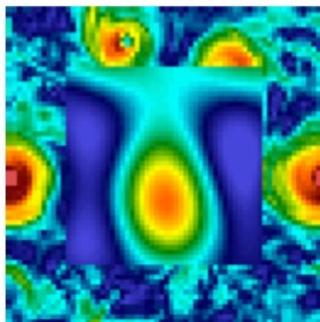
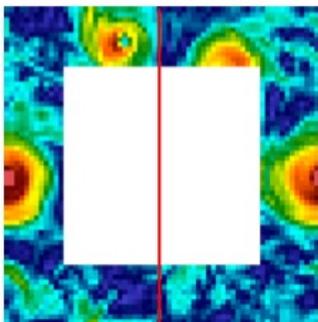
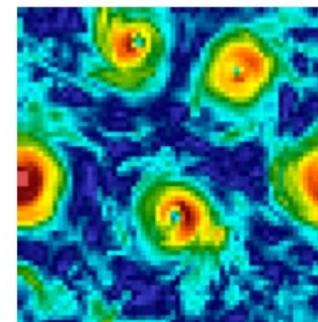
EPOD



GAN



Original



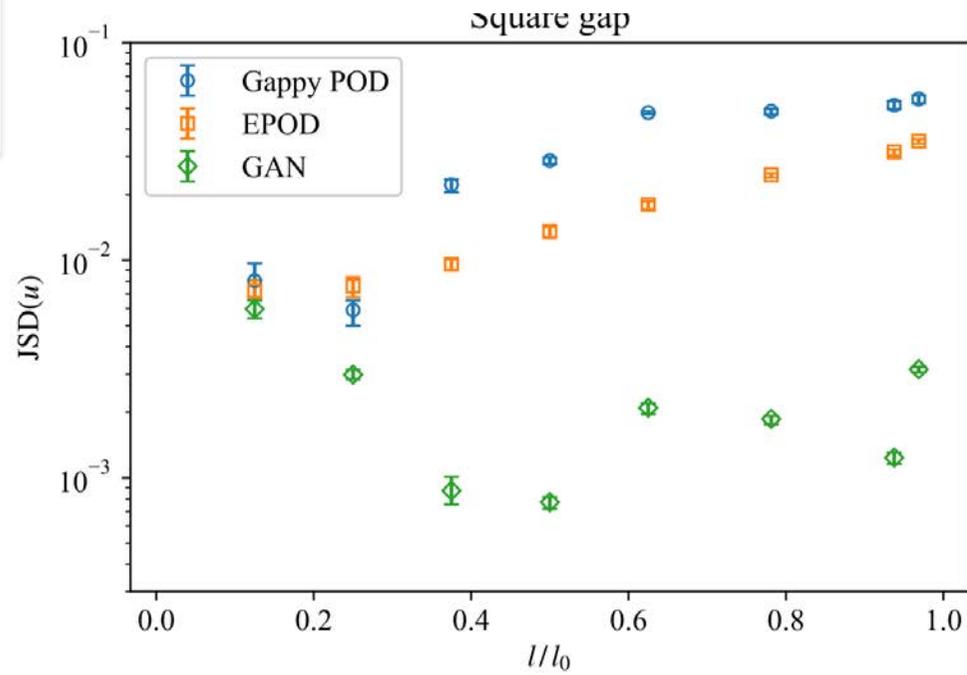
$$D(P \parallel Q) = \int_{-\infty}^{\infty} P(x) \log \left(\frac{P(x)}{Q(x)} \right) dx$$

$$M = \frac{1}{2}(P + Q)$$

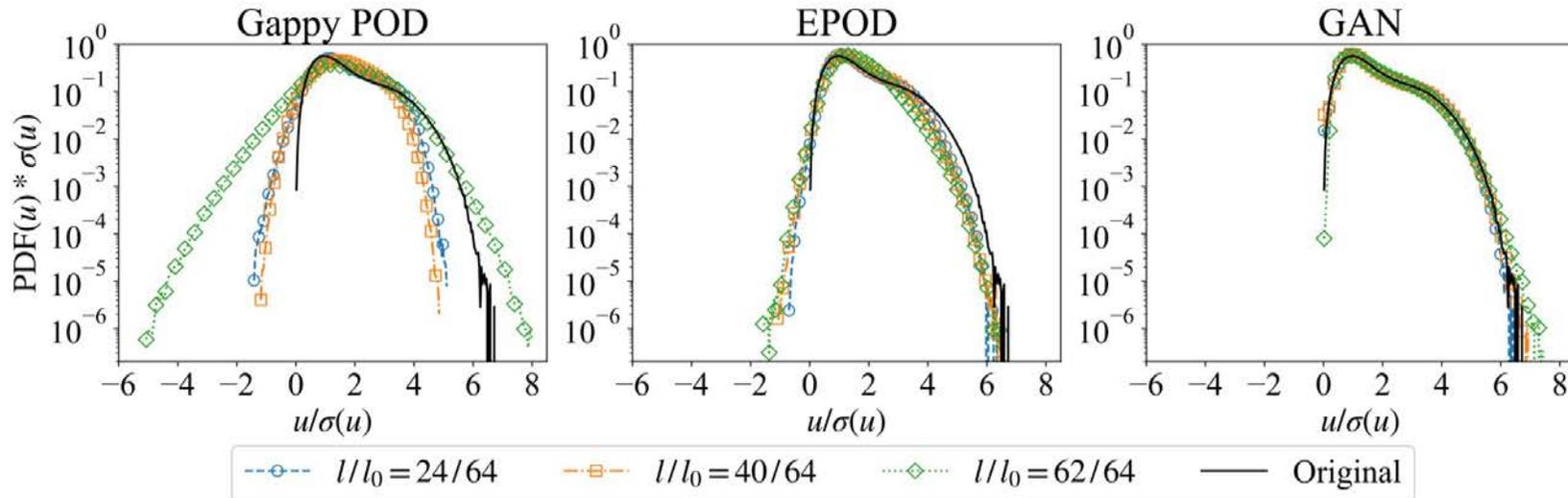
JENSEN-SHANNON

$$\rightarrow \text{JSD}(P \parallel Q) = \frac{1}{2}D(P \parallel M) + \frac{1}{2}D(Q \parallel M),$$

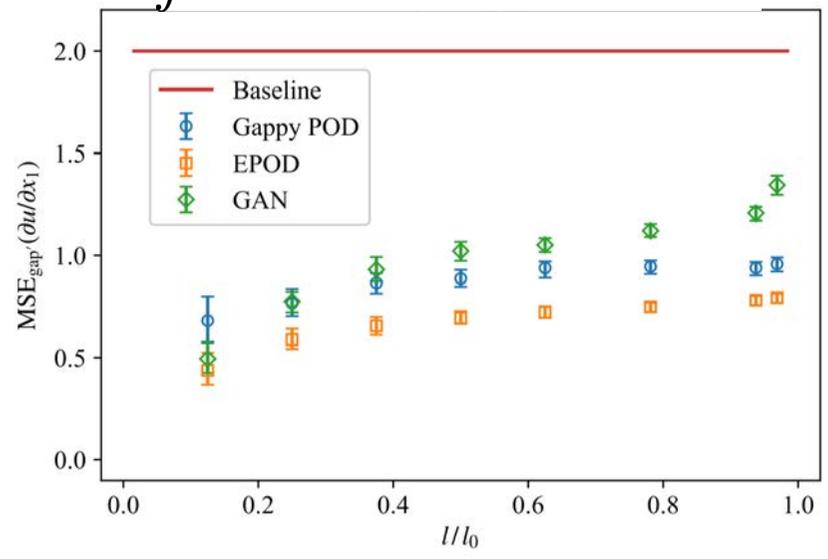
KULLBACK-LEIBLER



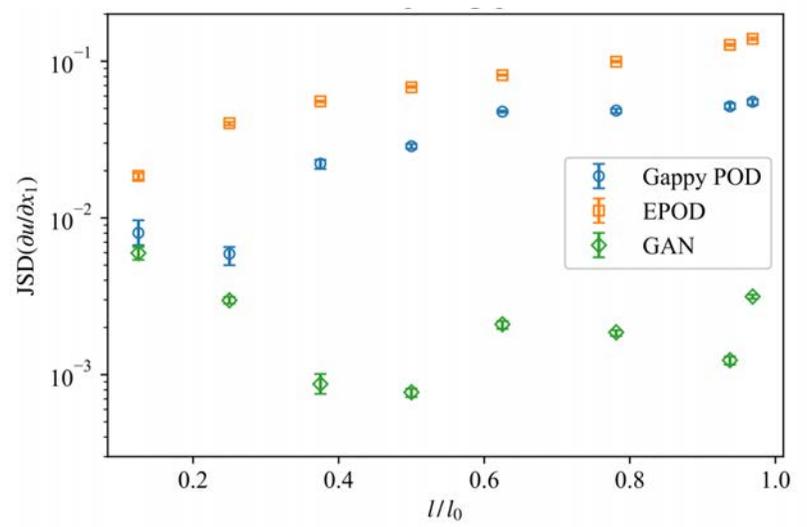
11



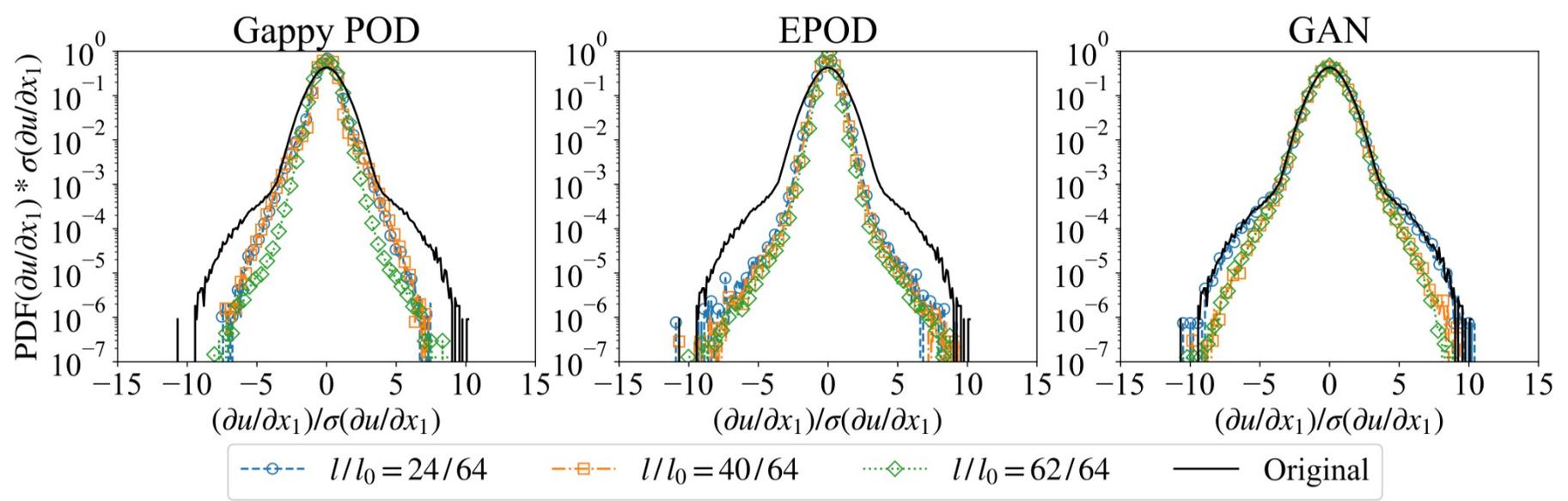
$$\int d\mathbf{x} [\partial_x u^p(\mathbf{x}, \theta) - \partial_x u^t(\mathbf{x})]^2$$



$$JSD(P \parallel Q) = \frac{1}{2}D(P \parallel M) + \frac{1}{2}D(Q \parallel M),$$



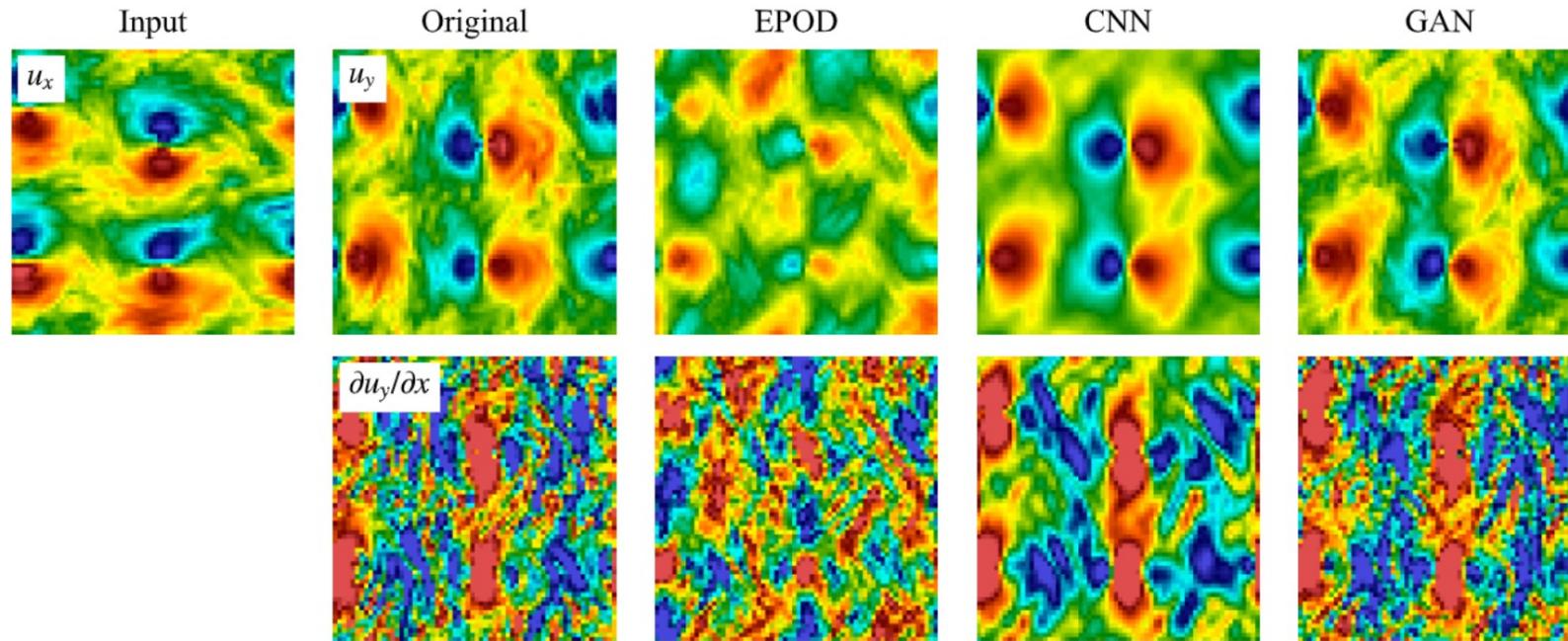
15



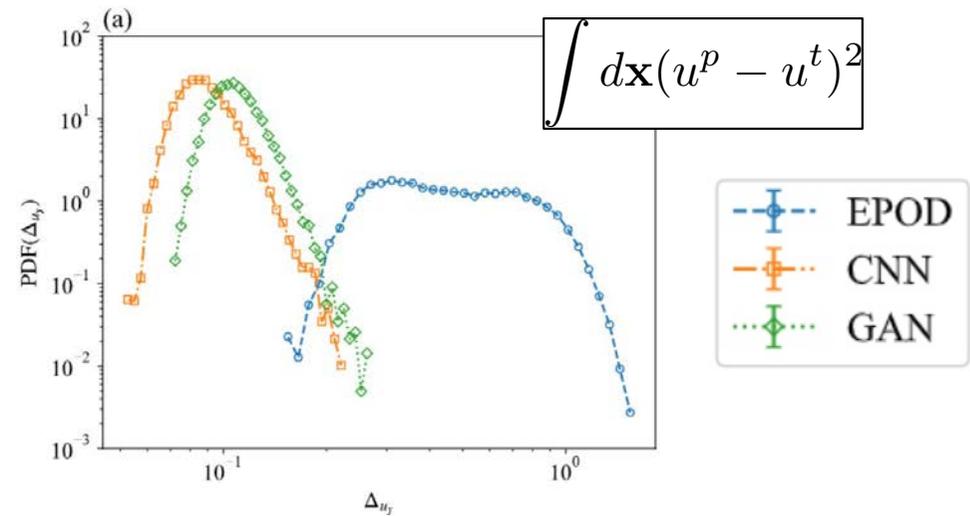
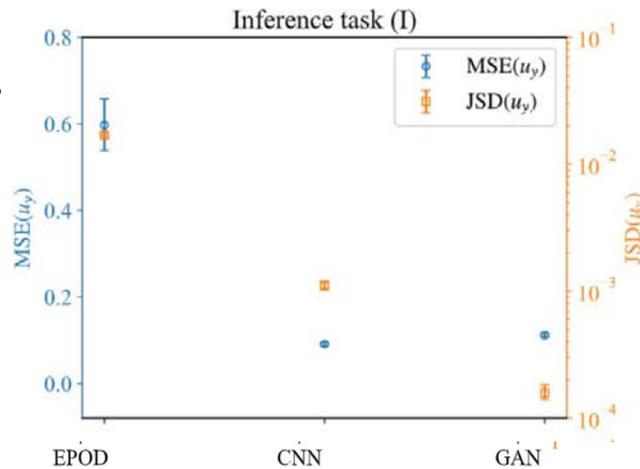
Generative adversarial networks to infer velocity components in rotating turbulent flows

Tianyi Li , Michele Buzzicotti, Luca Biferale & Fabio Bonaccorso

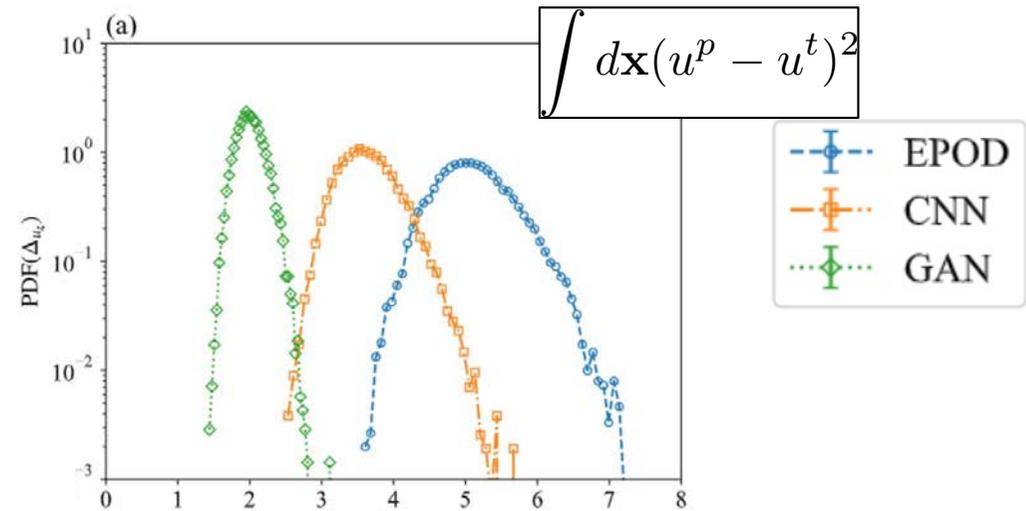
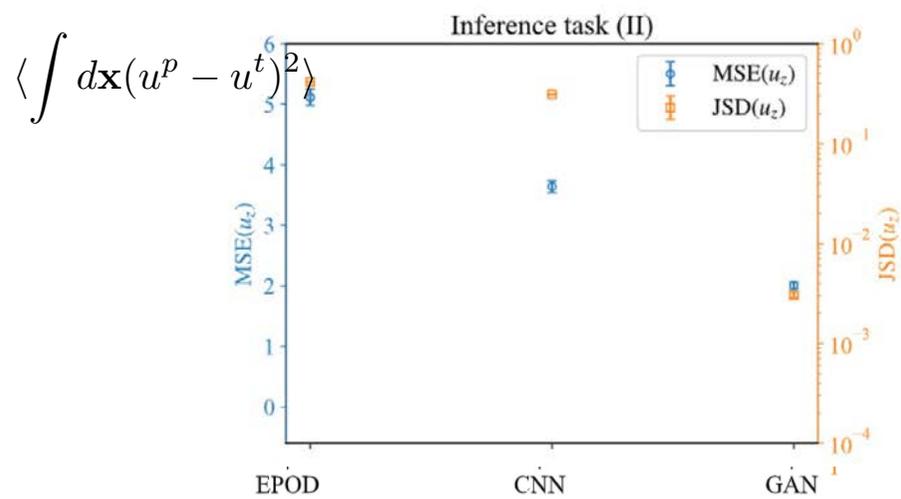
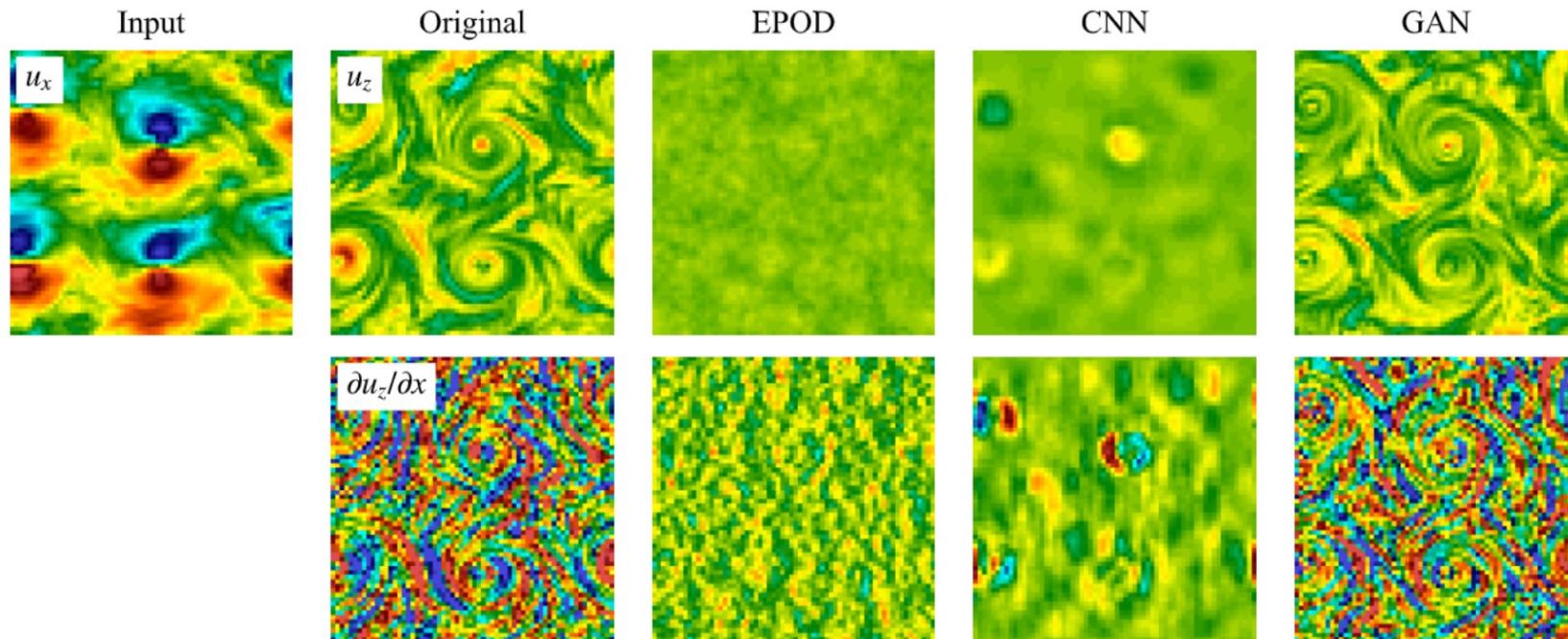
The European Physical Journal E **46**, Article number: 31 (2023)



$$\langle \int d\mathbf{x} (u^p - u^t)^2 \rangle$$



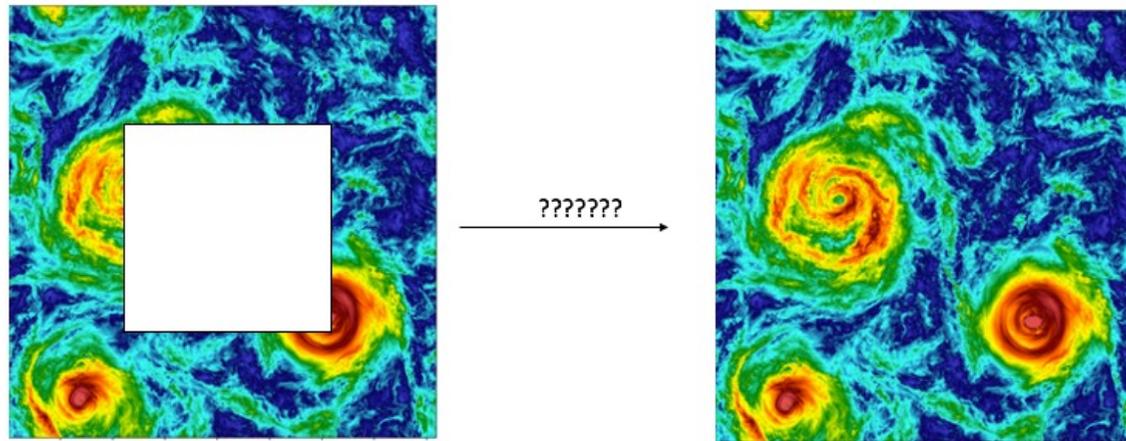
Generative Adversarial Networks to infer velocity components in rotating turbulent flows



NUDGING: AN EQUATION-INFORMED UNBIASED TOOL TO ASSIMILATE AND RECONSTRUCT TURBULENCE DATA/PHYSICS BY ADDING A DRAG TERM AGAINST PARTIAL FIELD MEASUREMENTS

EQUATIONS
BASED

C.C. Lalescu, C. Meneveau and G.L. Eyink. Synchronization of Chaos in Fully Developed Turbulence. Phys. Rev. Lett. 110, 084102 (2013)
 A.Farhat, E. Lunasin, and E.S. Titi. Abridged Continuous Data Assimilation for the 2d Navier-Stokes Equations Utilizing Measurements of Only One Component of the Velocity Field. J. Math. Fluid Mech. 18(1), 1 (2016)
Patricio Clark Di Leoni, Andrea Mazzino, and L.B. Synchronization to Big Data: Nudging the Navier-Stokes Equations for Data Assimilation of Turbulent Flows Phys. Rev. X 10, 011023 (2020)



FULLY PHYSICS COMPLIANT 🤔

NEED HUGE COMPUTATIONAL RESOURCES 😞

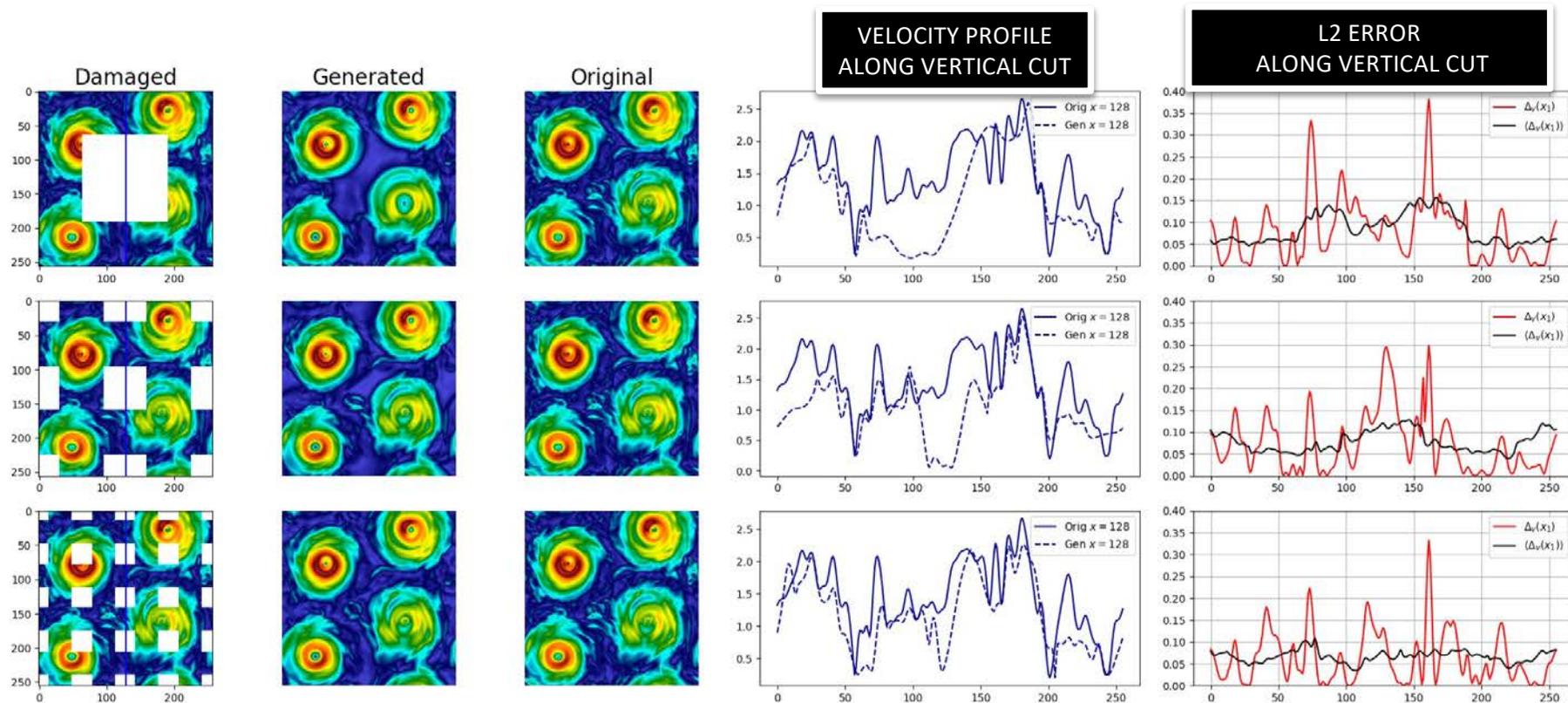
$$\mathbf{v}_N = G[\mathbf{v}_{true}]$$

$$\mathbf{v}_{true}$$

$$\begin{cases} \partial_t \mathbf{v} + \mathbf{v} \cdot \partial_x \mathbf{v} + \partial_x P - \nu \Delta \mathbf{v} = 2\mathbf{v} \times \boldsymbol{\Omega} + \mathcal{S}\mathbf{v} + \alpha g \hat{\mathbf{z}} T + \mathcal{F} - N(\mathbf{v}_N - \mathbf{v}) \\ \partial_x \mathbf{v} = 0 \end{cases}$$

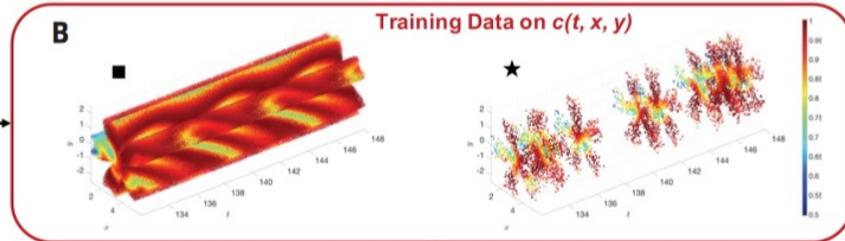
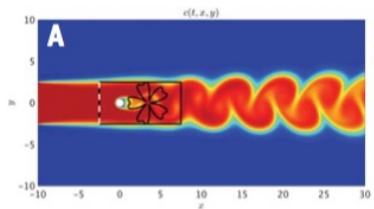
NO NEED TO TRAIN!! NAVIER AND STOKES DID THE JOB FOR YOU: ONE CONF IS ENOUGH

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} + 2\Omega \hat{x}_3 \times \mathbf{v} = -\nabla p + \nu \nabla^2 \mathbf{v} + \gamma(1 - \hat{M})_{x_3} \odot (\mathbf{v} - \mathbf{v}_{\text{ref}})$$

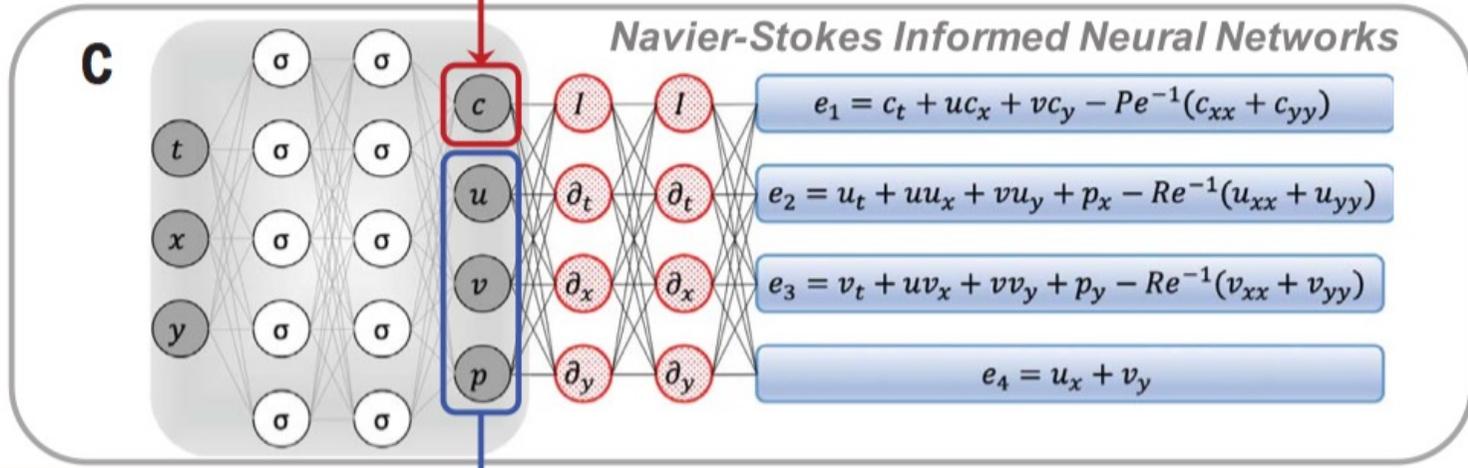


Synchronization to Big Data: Nudging the Navier-Stokes Equations for Data Assimilation of Turbulent Flows
 Patricio Clark Di Leoni, Andrea Mazzino, and L. B. Phys. Rev. X **10**, 011023 (2020)

Reconstruction of turbulent data with deep generative models for semantic inpainting from TURB-Rot database
 M. Buziccotti, F. Bonaccorso, P. Clark Di Leoni, and L. B. Phys. Rev. Fluids **6**, 050503 (2021)



PHYSICS INFORMED



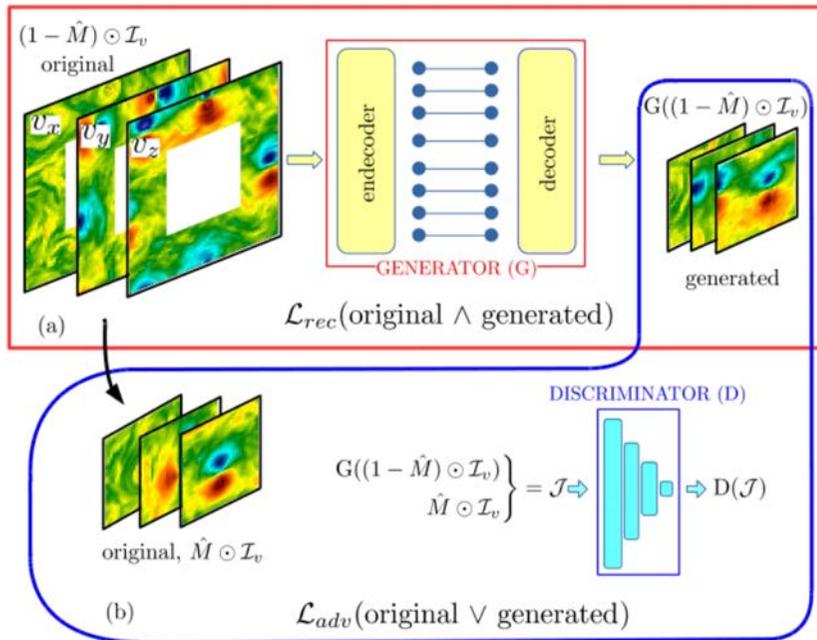
$$MSE = \frac{1}{N} \sum_{n=1}^N |c(t^n, x^n, y^n, z^n) - c^n|^2 + \sum_{i=1}^5 \frac{1}{M} \sum_{m=1}^M |e_i(t^m, x^m, y^m, z^m)|^2$$

ML-TRAINED ON A SPARSE SPATIO+TEMPORAL DATASET FOR CONCENTRATION -> INFER VELOCITY + PRESSURE -> BACK PROPAGATE FOR GRADIENTS (AUTOMATIC DIFFERENTIATION)-> NAVIER-STOKES

Hidden fluid mechanics: Learning velocity and pressure fields from flow visualizations. M. Raissi A. Yazdani , G. E. Karniadakis , Science 367, 1026–1030 (2020)

Physics-Informed Neural Network for Ultrasound Nondestructive Quantification of Surface Breaking Cracks K. Shukla, P. Clark Di Leoni, J. Blackshire, D. Sparkman & G. E. Karniadakis Journal of Nondestructive Evaluation 39 (2020)

CONTEXT ENCODER



CNN-GAN

-EQUATION-FREE

GENERATION OF MISSING DATA ONLY

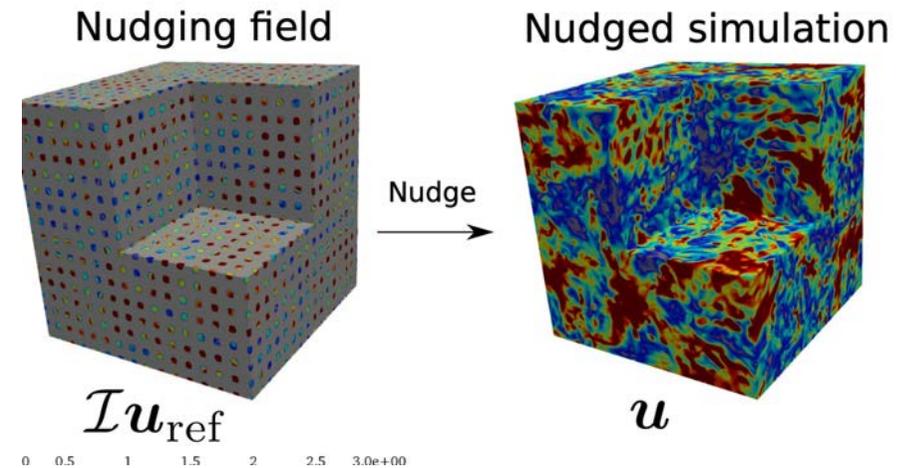
+ONCE TRAINED -> INSTANTANEOUS

+MIXED INPUT FEATURES

LINEAR CASE: EXTENDED-POD

NUDGING

$$\begin{cases} \partial_t \mathbf{v} + \mathbf{v} \cdot \partial_x \mathbf{v} + \partial_x P - \nu \Delta \mathbf{v} = 2\mathbf{v} \times \boldsymbol{\Omega} + \mathcal{S}\mathbf{v} + \alpha g \hat{\mathbf{z}} T + \mathcal{F} - N(\mathbf{v}_N - \mathbf{v}) \\ \partial_t T + \mathbf{v} \cdot \partial_x T - \chi \Delta T = \mathcal{G}v_z + \mathcal{L} - N_T(T_N - T) \end{cases}$$



+EQUATION-INFORMED

GENERATION OF FRAME & MISSING DATA

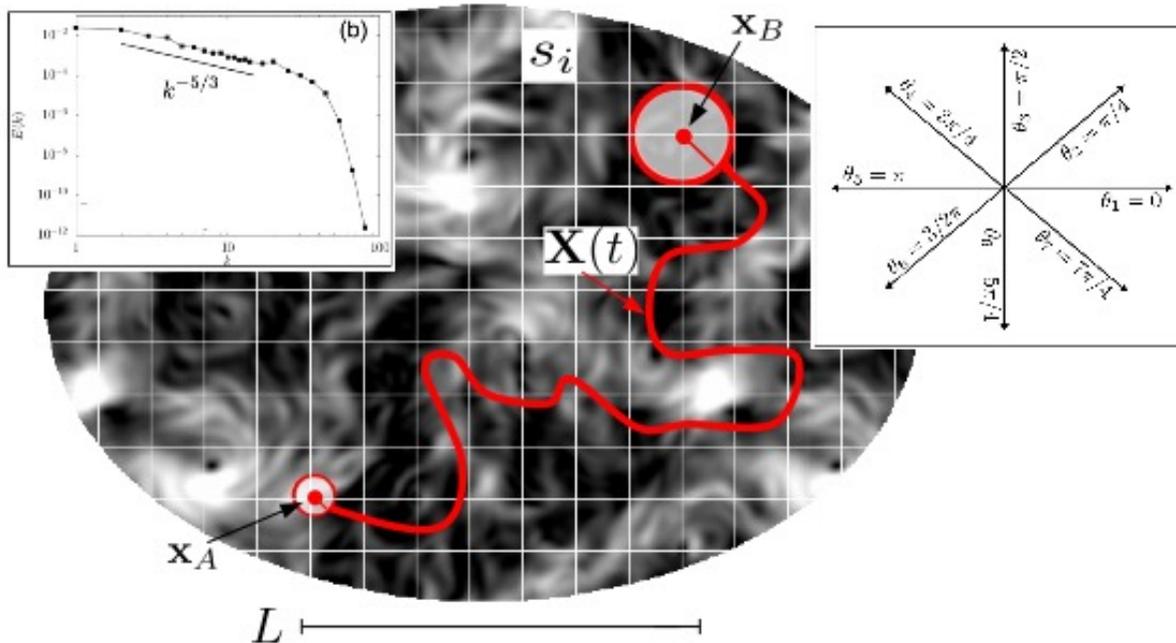
-NEW 3D DNS FOR EACH DA

-RESTRICTED INPUT FEATURES

Zermelo's problem: Optimal point-to-point navigation in 2D turbulent flows using Reinforcement Learning

L. Biferale,¹ F. Bonaccorso,^{1,2} M. Bucciotti,¹ P. Clark Di Leoni,^{1,3} and K. Gustavsson⁴

Chaos: An Interdisciplinary Journal of Nonlinear Science
29.10 (2019): 103138.
arXiv preprint:1907.08591



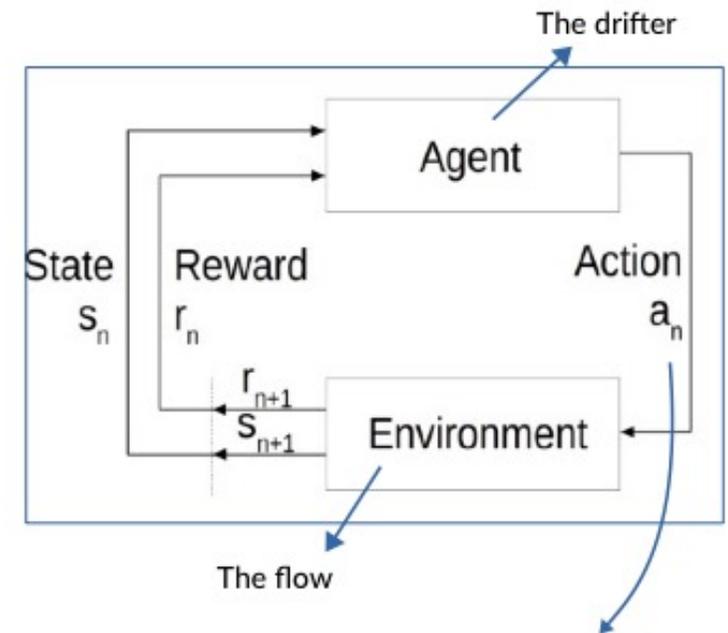
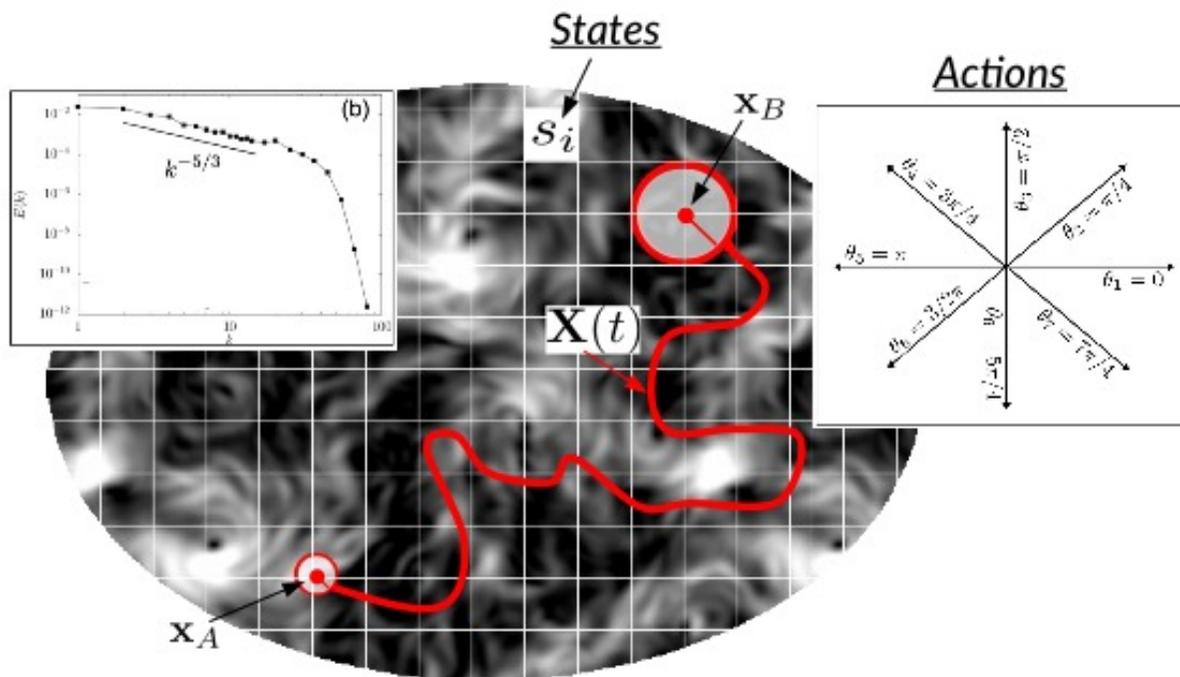
$$\begin{cases} \dot{\mathbf{X}}_t = \mathbf{u}(\mathbf{X}_t) + \mathbf{U}^{ctrl}(\mathbf{X}_t) \\ \mathbf{U}^{ctrl}(\mathbf{X}_t) = V_s \mathbf{n}(\mathbf{X}_t) \end{cases}$$

$$\mathbf{n}(\mathbf{X}_t) = (\cos[\theta_t], \sin[\theta_t]),$$

$V_s \rightarrow$ Navigation speed is small compared to the velocity of the underling flow!

E. Zermelo, "Über das navigationsproblem bei ruhender oder veränderlicher windverteilung," ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik **11**, 114-124 (1931).
A. E. Bryson and Y. Ho, *Applied optimal control: optimization, estimation and control* (New York: Routledge, 1975).

Reinforcement Learning; Policy Gradient Methods



Parameterized policy:

$$\pi(a_j | s_i, \mathbf{q}) = \frac{\exp h(s_i, a_j, \mathbf{q})}{\sum_{k=1}^{N_a} \exp h(s_i, a_k, \mathbf{q})}$$

Parameterized state value function:

$$\hat{v}(s_i, \mathbf{w}) = \sum_{j=1}^{N_s} w_j \delta_{j,i}$$

Reward

$$r_t = -\Delta t$$

$$r_{tot} = -T_{A \rightarrow B}$$

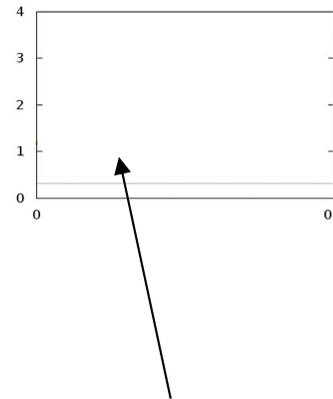
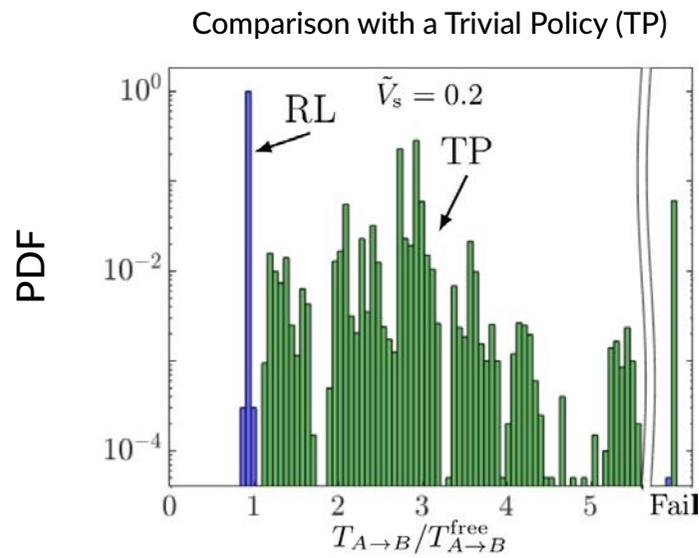
Actor-Critic algorithm

$$\begin{cases} \mathbf{q}_{t+\Delta t} = \mathbf{q}_t + \alpha_t \beta_t \nabla_{\mathbf{q}} \ln(\pi(a_t | s_t, \mathbf{q}_t)) \\ \mathbf{w}_{t+\Delta t} = \mathbf{w}_t + \alpha'_t \beta_t \nabla_{\mathbf{w}} \hat{v}(s_t, \mathbf{w}_t) \end{cases}$$

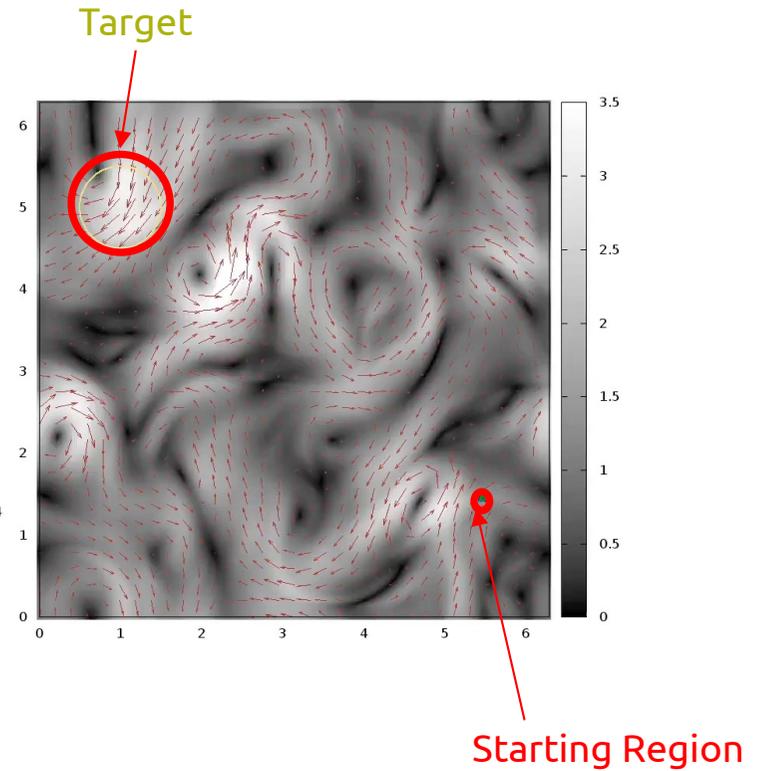
$$\beta_t = [\hat{r}_{t+\Delta t} - \hat{v}(s_t, \mathbf{w}_t)] \rightarrow \text{baseline}$$

TIME-DEPENDENT 2D TURBULENT FLOWS

REINFORCEMENT LEARNING (BLUE) VS TRIVIAL POLICY (GREEN) $\tilde{V}_s = 0.2$

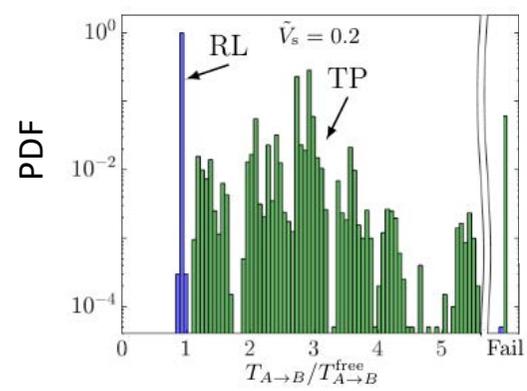
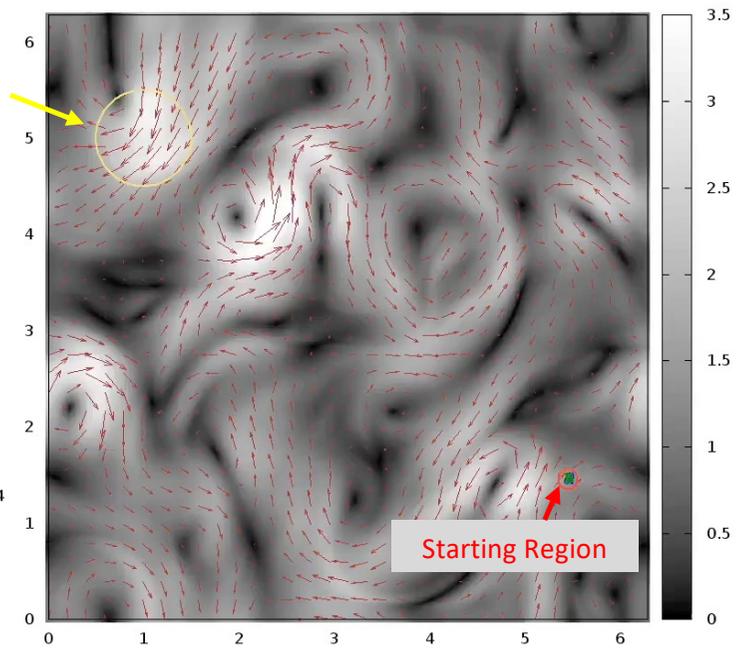
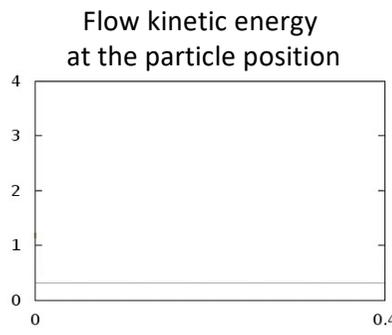
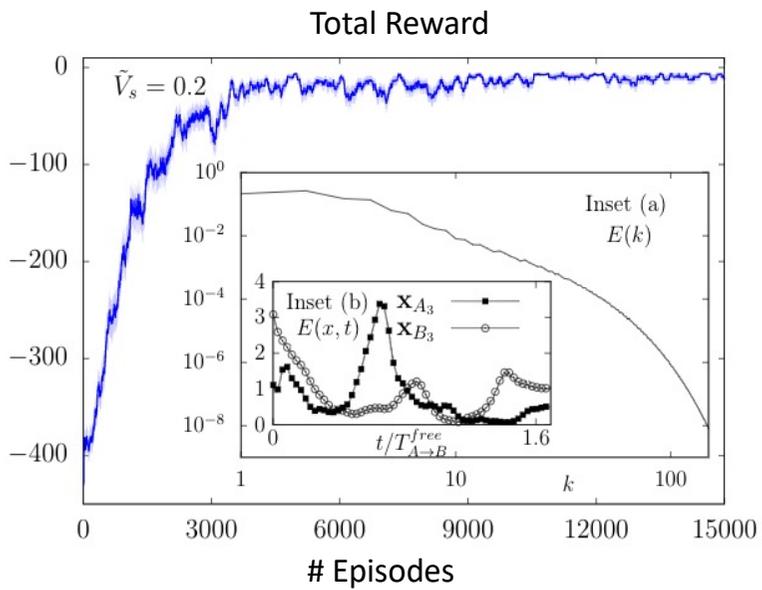


Flow kinetic energy
at the particle position



Time-Dependent 2D Turbulent Flow

$$\frac{V_s}{\max(u)} \sim 0.2$$

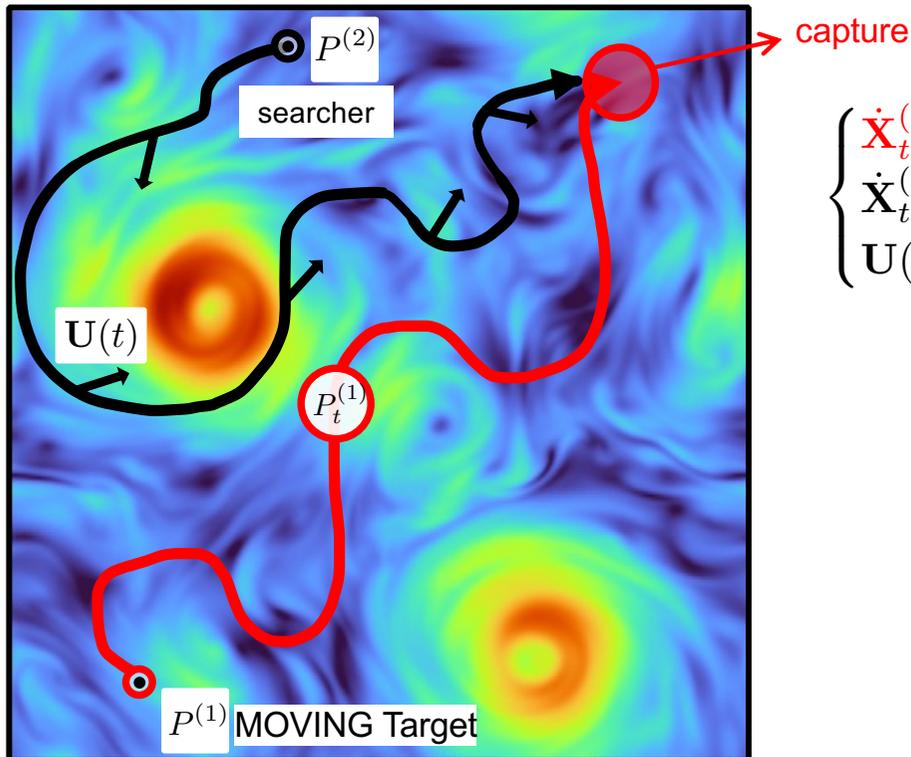


Reinforcement Learning (blue)
vs
Trivial Policy (green)

Catching a drifting target in turbulence via Optimal Control

C. Calascibetta,¹ L. Biferale,¹ F. Borra,² A. Celani,³ and M. Cencini⁴

2 AGENTS



Problem setup

$$\begin{cases} \dot{\mathbf{X}}_t^{(1)} = \mathbf{v}(\mathbf{X}_t^{(1)}, t) \\ \dot{\mathbf{X}}_t^{(2)} = \mathbf{v}(\mathbf{X}_t^{(2)}, t) + \mathbf{U}(t) \\ \mathbf{U}(t) = V_s \hat{\mathbf{n}}(t) \end{cases} \longrightarrow \mathbf{U}(t) = ?$$

$$\hat{\mathbf{n}}(t) = (\cos[\theta_t], \sin[\theta_t])$$

Tools:

- (1) Heuristic policies
- (2) Optimal Control (OC) theory
- (3) Reinforcement Learning (RL)

Goal: minimize the separation/capture
in a finite time-horizon

(2) Optimal Control theory – Pontryagin minimum principle

state variables control variables

Minimize $J = C_F(\mathbf{X}(t_f)) + \int_{t_0}^{t_f} dt [L(\mathbf{X}(t), \mathbf{U}(t), t)]$
performance index Lagrangian function

Imposing $\dot{\mathbf{X}}_t = \mathbf{f}(\mathbf{X}(t), \mathbf{U}(t), t)$
 and other possible constraints,
 e.g.: $\begin{cases} \mathbf{X}(t_f) = \mathbf{X}_*, & \mathbf{X}(t_0) \leq \mathbf{X}_*, \\ \|\mathbf{U}(t)\|^2 = 1, & \|\mathbf{U}(t)\|^2 \leq 1, \text{ exc.} \end{cases}$

- **Model based** and analytical tool
- Perfect knowledge required

$$\|\mathbf{R}_{t_0}\| \sim \frac{V_s}{\lambda_{lyapunov}} \text{ border of controllability}$$

In our case:

capture's distance

$$\|\mathbf{R}^*\| = \|\mathbf{R}_{t_0}\|/100$$

Minimize $J = \|\mathbf{R}_{t_f}\|^2 + c \int_{t_0}^{t_f} dt \theta(\|\mathbf{R}_{t_f}\|^2 - \|\mathbf{R}^*\|^2)$

Imposing (2) and the control constraint $\|\hat{\mathbf{n}}(t)\|^2 = 1$

$$\begin{cases} \dot{\mathbf{R}}_t = \nabla v_t \mathbf{R}_t + \mathbf{U}(t), \\ \mathbf{U}(t) = V_S \hat{\mathbf{n}}(t). \end{cases} \quad (2)$$

LINEAR REGIME

Optimal Control theory to minimize Lagrangian particles dispersion in turbulent flows

Constrained performance index:

$$\tilde{J} = \|\mathbf{R}_{t_f}\|^2 + \underbrace{\int_{t_0}^{t_f} dt \{c[\theta(\|\mathbf{R}_t\|^2 - \|\mathbf{R}^*\|^2)] + \boldsymbol{\lambda}^T(t)[\nabla \mathbf{v}_t \mathbf{R}_t + V_s \hat{\mathbf{n}}(t) - \dot{\mathbf{R}}] + \mu(t)(1 - \|\hat{\mathbf{n}}(t)\|^2)\}}_{\text{Constrained minimization problem}}$$

Constrained minimization problem

Integrating by parts,

$$\tilde{J} = \|\mathbf{R}_{t_f}\|^2 - \boldsymbol{\lambda}^T(t_f) \mathbf{R}_{t_f} + \boldsymbol{\lambda}^T(t_0) \mathbf{R}_{t_0} + \int_{t_0}^{t_f} dt [H(\mathbf{R}_t, \boldsymbol{\lambda}(t), \hat{\mathbf{n}}(t), \mu(t), t) + \dot{\boldsymbol{\lambda}}^T \mathbf{R}_t],$$

$$H(\mathbf{R}_t, \boldsymbol{\lambda}(t), \hat{\mathbf{n}}(t), \mu(t), t) = c[\theta(\|\mathbf{R}_t\|^2 - \|\mathbf{R}^*\|^2)] + \boldsymbol{\lambda}^T(t)[\nabla \mathbf{v}_t \mathbf{R}_t + V_s \hat{\mathbf{n}}(t)] + \mu(t)(1 - \|\hat{\mathbf{n}}(t)\|^2). \quad \text{Hamiltonian function}$$

Consider variation in \tilde{J} :

$$\delta \tilde{J} = \left[(\mathbf{R}_t - \boldsymbol{\lambda}^T(t)) \delta \mathbf{R} \right]_{t=t_f} + \left[\boldsymbol{\lambda}^T(t) \delta \mathbf{R} \right]_{t=t_0} + \int_{t_0}^{t_f} dt \left\{ \left[\frac{\partial H}{\partial \mathbf{R}} + \dot{\boldsymbol{\lambda}}^T \right] \delta \mathbf{R} + \frac{\partial H}{\partial \hat{\mathbf{n}}} \delta \hat{\mathbf{n}} \right\}$$

Euler-Lagrange equations:	$\begin{cases} \dot{\boldsymbol{\lambda}} = -\frac{\partial H}{\partial \mathbf{R}} = -2c \mathbf{R}_t \delta(\ \mathbf{R}_t\ ^2 - \ \mathbf{R}^*\ ^2) - (\nabla \mathbf{v}_t)^T \boldsymbol{\lambda}(t), \\ \boldsymbol{\lambda}(t_f) = 2\mathbf{R}_{t_f}, \\ \frac{\partial H}{\partial \hat{\mathbf{n}}} = 0 \implies \hat{\mathbf{n}}(t) = \frac{V_s \boldsymbol{\lambda}(t)}{2\mu(t)} = -\frac{\boldsymbol{\lambda}(t)}{\ \boldsymbol{\lambda}(t)\ }. \end{cases}$	$\begin{cases} \dot{\mathbf{R}}_t = \nabla \mathbf{v}_t \mathbf{R}_t + \mathbf{U}(t), \\ \mathbf{R}_{t_0} = \text{given}, \\ \mathbf{U}(t) = V_s \hat{\mathbf{n}}(t). \end{cases}$
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Optimal Control theory to minimize Lagrangian particles dispersion in turbulent flows

Euler-Lagrange equations:

$$\left\{ \begin{array}{l} \dot{\lambda} = -\frac{\partial H}{\partial \mathbf{R}} = -2c \mathbf{R}_t \delta(\|\mathbf{R}_t\|^2 - \|\mathbf{R}^*\|^2) - (\nabla \mathbf{v}_t)^T \boldsymbol{\lambda}(t), \\ \boldsymbol{\lambda}(t_f) = 2\mathbf{R}_{t_f}, \\ \frac{\partial H}{\partial \hat{\mathbf{n}}} = 0 \implies \hat{\mathbf{n}}(t) = \frac{V_s \boldsymbol{\lambda}(t)}{2\mu(t)} = -\frac{\boldsymbol{\lambda}(t)}{\|\boldsymbol{\lambda}(t)\|}. \end{array} \right.$$

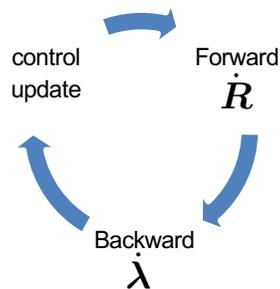
backward integration

$$\left\{ \begin{array}{l} \dot{\mathbf{R}}_t = \nabla \mathbf{v}_t \mathbf{R}_t + \mathbf{U}(t), \\ \mathbf{R}_{t_0} = \text{given}, \\ \mathbf{U}(t) = V_S \hat{\mathbf{n}}(t). \end{array} \right.$$

Forward integration

computationally heavy

It requires iterative searching with backward and forward integration such as to identify the optimal control



$$\begin{cases} \dot{\mathbf{X}}_t^{(1)} = \mathbf{v}(\mathbf{X}_t^{(1)}, t) \\ \dot{\mathbf{X}}_t^{(2)} = \mathbf{v}(\mathbf{X}_t^{(2)}, t) + \mathbf{U}(t) \\ \mathbf{U}(t) = V_s \hat{\mathbf{n}}(t) \end{cases}$$

$$\mathbf{U}(t) = ?$$

$$\begin{cases} \mathbf{R}_t = \mathbf{X}_t^{(2)} - \mathbf{X}_t^{(1)} \\ L = \text{characteristic scale of the flow} \end{cases}$$

(1) (semi) Heuristic policies

Trivial Policy: constantly chooses the direction that points towards the moving target

$$\hat{\mathbf{n}}(t) = -\hat{\mathbf{R}}_t$$

Surfing policy*: valid at large scales, i.e., $\|\mathbf{R}_t\| \gg L$. Based on a free parameter τ_s .

Perturbative policy: valid at small scales, i.e. $\|\mathbf{R}_t\| \ll L$. Based on a free parameter τ_p .

*Monthiller, Rémi, et al. **Surfing on Turbulence: A Strategy for Planktonic Navigation.** *Phys. Rev. Lett.* **129**, 064502 (2022)

$$\begin{cases} \dot{\mathbf{X}}_t^{(1)} = \mathbf{v}(\mathbf{X}_t^{(1)}, t) \\ \dot{\mathbf{X}}_t^{(2)} = \mathbf{v}(\mathbf{X}_t^{(2)}, t) + \mathbf{U}(t) \\ \mathbf{U}(t) = V_s \hat{\mathbf{n}}(t) \end{cases}$$

$$\mathbf{U}(t) = ?$$

$$\begin{cases} \mathbf{R}_t = \mathbf{X}_t^{(2)} - \mathbf{X}_t^{(1)} \\ L = \text{characteristic scale of the flow} \end{cases}$$

(1) (semi) Heuristic policies

Surfing policy* - derivation

- Approximate linearly the underlying flow, $\mathbf{v}(\mathbf{X}_t^{(2)}, t)$ for $t_0 < t < \tau_s$; (Assuming constant gradients for a time τ_s)

$$\dot{\mathbf{X}}_t^{(2)} = \mathbf{v}_{t_0} + (\nabla \mathbf{v})_{t_0} \cdot (\mathbf{X}_t^{(2)} - \mathbf{X}_{t_0}^{(2)}) + \left(\frac{\partial \mathbf{v}}{\partial t} \right)_{t_0} (t - t_0) + \mathbf{U}(t),$$

- Find $\mathbf{U}(t)$ such that $-(\mathbf{X}_{\tau_s}^{(2)} - \mathbf{X}_{t_0}^{(2)}) \cdot \hat{\mathbf{R}}_{t_0}$ is maximum;

$$\hat{\mathbf{n}}(t) = - \frac{[e^{(\tau_s - t) \nabla \mathbf{v}_{t_0}}]^T \cdot \hat{\mathbf{R}}_{t_0}}{\| [e^{(\tau_s - t) \nabla \mathbf{v}_{t_0}}]^T \cdot \hat{\mathbf{R}}_{t_0} \|}$$

(Assuming constant the direction $\hat{\mathbf{R}}_t$ for a time τ_s)

$$\downarrow \\ \|\mathbf{R}_t\| \gg L$$

- Numerically optimize the free parameter τ_s .

* Monthiller, Rémi, et al. Surfing on Turbulence: A Strategy for Planktonic Navigation. *Phys. Rev. Lett.* **129**, 064502 (2022)

$$\dot{\mathbf{X}}_t^{(2)} = \mathbf{v}_{t_0} + (\nabla \mathbf{v})_{t_0} \cdot (\mathbf{X}_t^{(2)} - \mathbf{X}_{t_0}^{(2)}) + \left(\frac{\partial \mathbf{v}}{\partial t} \right)_{t_0} (t - t_0) + V_s \hat{\mathbf{n}}(t)$$

$$\begin{aligned} \mathbf{X}_{\tau_s}^{(2)} = & \mathbf{X}_{t_0}^{(2)} + [e^{\tau_s (\nabla \mathbf{v})_{t_0}} - \mathbb{I}] \cdot (\nabla \mathbf{v}_{t_0})^{-1} \cdot \left[\mathbf{v}_{t_0} + (\nabla \mathbf{v}_{t_0})^{-1} \cdot \left(\frac{\partial \mathbf{v}}{\partial t} \right)_{t_0} \right] - \\ & - \tau_s (\nabla \mathbf{v}_{t_0})^{-1} \cdot \left(\frac{\partial \mathbf{v}}{\partial t} \right)_{t_0} + V_s \int_{t_0}^{\tau_s} dt e^{(\tau_s - t) \nabla \mathbf{v}_{t_0}} \cdot \hat{\mathbf{n}}(t) \end{aligned}$$

find $\hat{\mathbf{n}}(t)$ such as $-(\mathbf{X}_{\tau_s}^{(2)} - \mathbf{X}_{t_0}^{(2)}) \cdot \hat{\mathbf{R}}_{t_0}$ is maximum,

means find $\hat{\mathbf{n}}(t)$ such that $-\int_{t_0}^{\tau_s} dt \underbrace{[e^{(\tau_s - t) \nabla \mathbf{v}_{t_0}} \cdot \hat{\mathbf{n}}(t) \cdot \hat{\mathbf{R}}_{t_0}]}_{-[e^{(\tau_s - t) \nabla \mathbf{v}_{t_0}}]^T \cdot \hat{\mathbf{R}}_{t_0} \cdot \hat{\mathbf{n}}(t)}$ is maximum (i.e. by maximizing the integrand).

$\hat{\mathbf{n}}(t)$ must be collinear to $-[e^{(\tau_s - t) \nabla \mathbf{v}_{t_0}}]^T \cdot \hat{\mathbf{R}}_{t_0}$ \longrightarrow

$$\hat{\mathbf{n}}(t) = - \frac{[e^{(\tau_s - t) \nabla \mathbf{v}_{t_0}}]^T \cdot \hat{\mathbf{R}}_{t_0}}{\| [e^{(\tau_s - t) \nabla \mathbf{v}_{t_0}}]^T \cdot \hat{\mathbf{R}}_{t_0} \|}$$

* Monthiller, Rémi, et al. **Surfing on Turbulence: A Strategy for Planktonic Navigation**. *Phys. Rev. Lett.* **129**, 064502 (2022)

$$\begin{cases} \dot{\mathbf{X}}_t^{(1)} = \mathbf{v}(\mathbf{X}_t^{(1)}, t) \\ \dot{\mathbf{X}}_t^{(2)} = \mathbf{v}(\mathbf{X}_t^{(2)}, t) + \mathbf{U}(t) \\ \mathbf{U}(t) = V_s \hat{\mathbf{n}}(t) \end{cases}$$

$$\mathbf{U}(t) = ?$$

$$\begin{cases} \mathbf{R}_t = \mathbf{X}_t^{(2)} - \mathbf{X}_t^{(1)} \\ L = \text{characteristic scale of the flow} \end{cases}$$

(1) (semi) Heuristic policies

Perturbative policy - derivation

- Consider linearity between the two agents, i.e., $\mathbf{v}(\mathbf{X}_t^{(2)}, t) \simeq \mathbf{v}(\mathbf{X}_t^{(1)}, t) + \nabla \mathbf{v}_t \mathbf{R}_t$, $\rightarrow \|\mathbf{R}_t\| \ll L$

$$\dot{\mathbf{R}}_t = \nabla \mathbf{v}_t \mathbf{R}_t + \mathbf{U}(t) \rightarrow \mathbf{R}_{\tau_p} = \underbrace{e^{[(\nabla \mathbf{v})_{t_0} \tau_p]} \mathbf{R}_{t_0}} + V_s \int_{t_0}^{\tau_p} dt e^{[(\nabla \mathbf{v})_{t_0} (\tau_p - t)]} \hat{\mathbf{n}}(t);$$

(Assuming constant gradients for a time τ_p)

- Find $\mathbf{U}(t)$ such that $\mathbf{R}_{\tau_p} \cdot \mathbf{R}_{\tau_p}^{free}$ is minimum;

$$\hat{\mathbf{n}}(t) = - \frac{[e^{(\tau_p - t) \nabla \mathbf{v}_{t_0}}]^T \cdot e^{(\nabla \mathbf{v})_{t_0} \tau_p} \cdot \hat{\mathbf{R}}_{t_0}}{\| [e^{(\tau_p - t) \nabla \mathbf{v}_{t_0}}]^T \cdot e^{(\nabla \mathbf{v})_{t_0} \tau_p} \cdot \hat{\mathbf{R}}_{t_0} \|}$$

- Numerically optimize the free parameter τ_p .

Optimal Control vs heuristic policies at **small scales**

Velocity field*

3D Direct Numerical Simulations $N = 1024^3$

$$\text{NSEs} \begin{cases} \partial_t \mathbf{v} = -\nabla p - (\mathbf{v} \cdot \nabla) \mathbf{v} + \nu \nabla^2 \mathbf{v} + \mathbf{F}, \\ \nabla \cdot \mathbf{v} = 0 \end{cases}$$

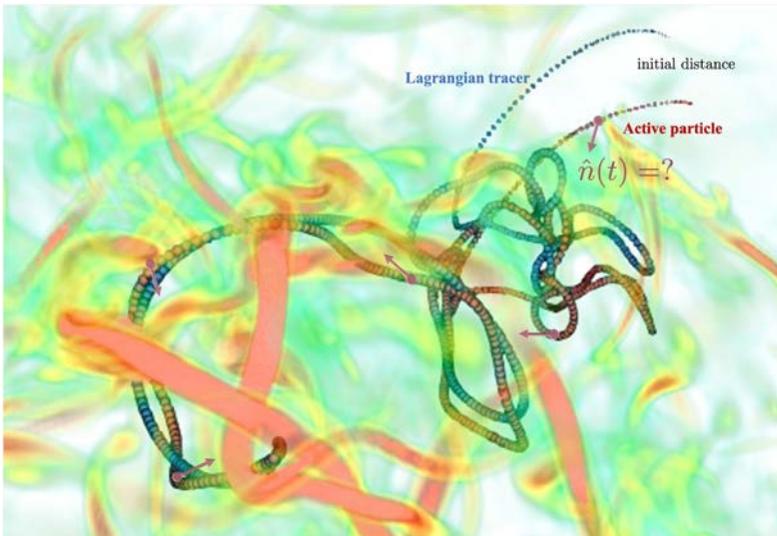
↓
homogeneous and
isotropic forcing

DNS parameters

$$\eta_k = 0.0043$$

$$\tau_\eta = 0.023$$

$$Re \simeq 17000$$



(1) **LINEAR REGIME** $\| \mathbf{R}_{t_0} \| < \eta_k$

$$\begin{cases} \dot{\mathbf{X}}_t^{(1)} = \mathbf{v}(\mathbf{X}_t^{(1)}, t) \\ \dot{\mathbf{X}}_t^{(2)} = \mathbf{v}(\mathbf{X}_t^{(2)}, t) + \mathbf{U}(t) \\ \mathbf{U}(t) = V_s \hat{\mathbf{n}}(t) \end{cases}$$

$$\mathbf{v}(\mathbf{X}_t^{(2)}, t) \simeq \mathbf{v}(\mathbf{X}_t^{(1)}, t) + \nabla \mathbf{v}_t \mathbf{R}_t$$

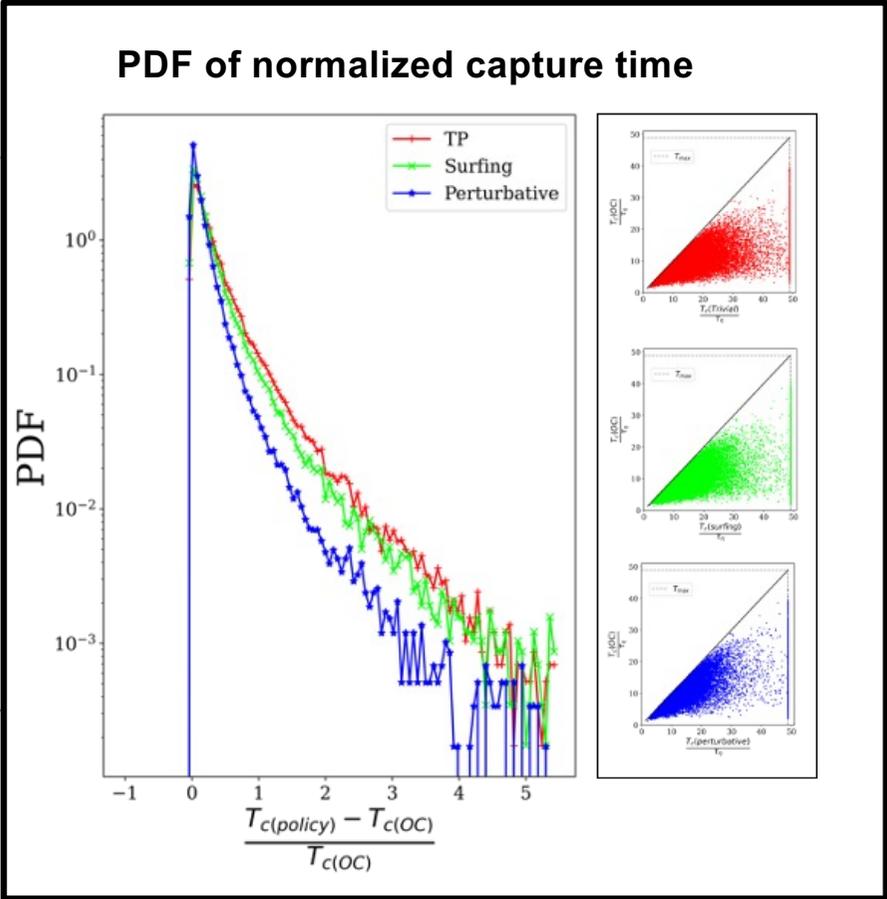
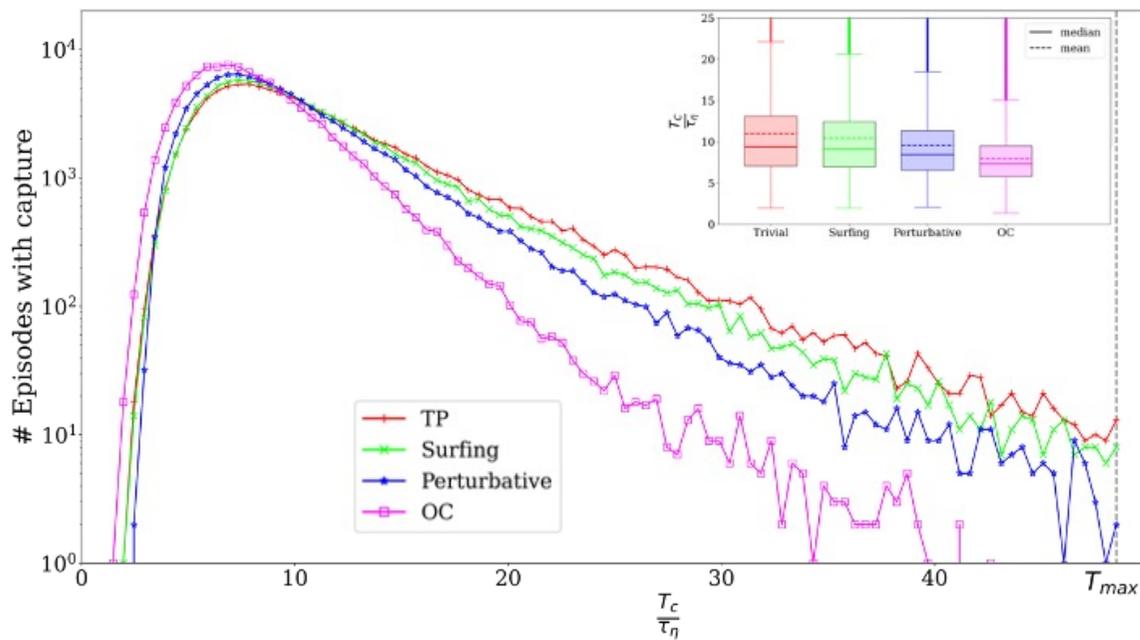
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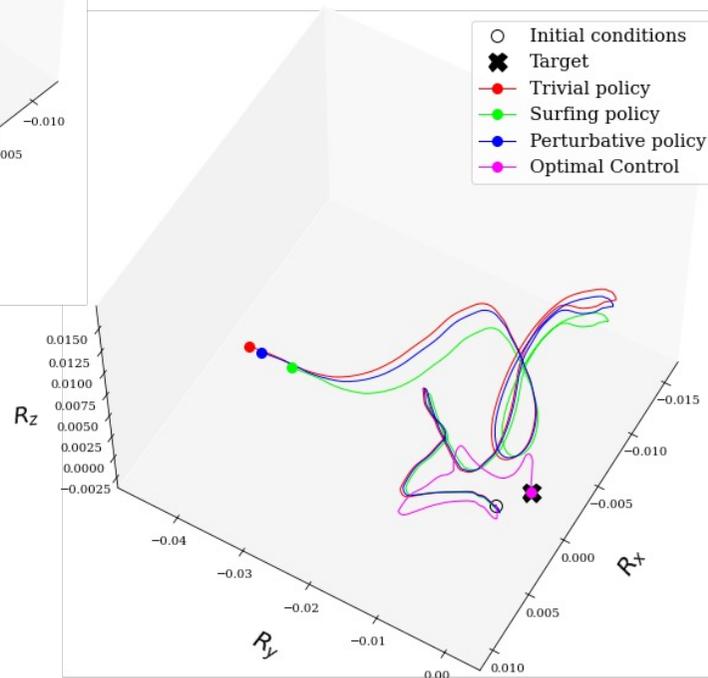
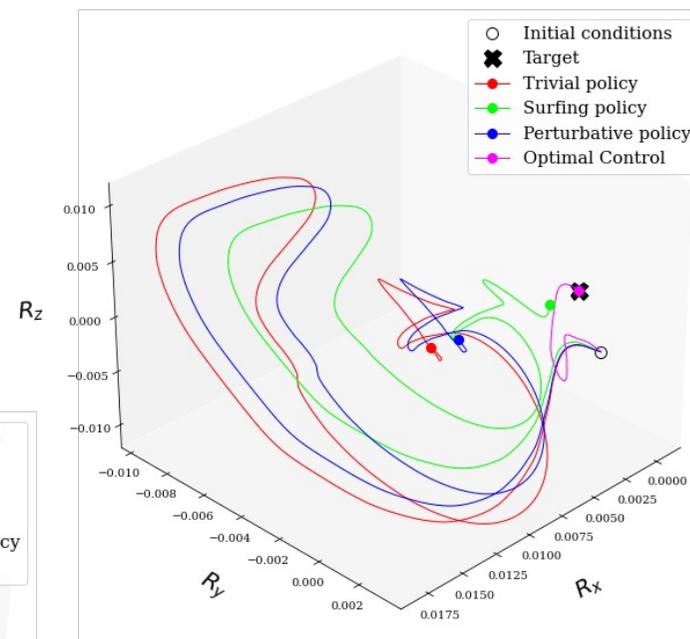
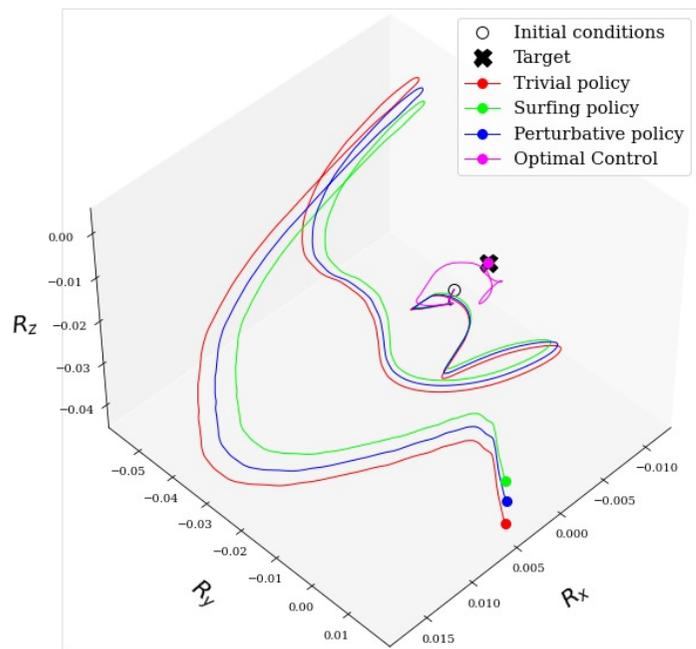
$$\dot{\mathbf{R}}_t = \nabla \mathbf{v}_t \mathbf{R}_t + \mathbf{U}(t)$$

Optimal Control vs heuristic policies in linear regime

$$\dot{R}_t = \nabla v_t R_t + U(t)$$

T_c = Capture time: (time of arrival at the desired distance)





pros & cons

Optimal Control

- + It is optimized
- It is model based and needs perfect information from the environment
- It is sensitive to variation of the initial condition
- It is difficult to consider a decision time in the control variable

Heuristic policies

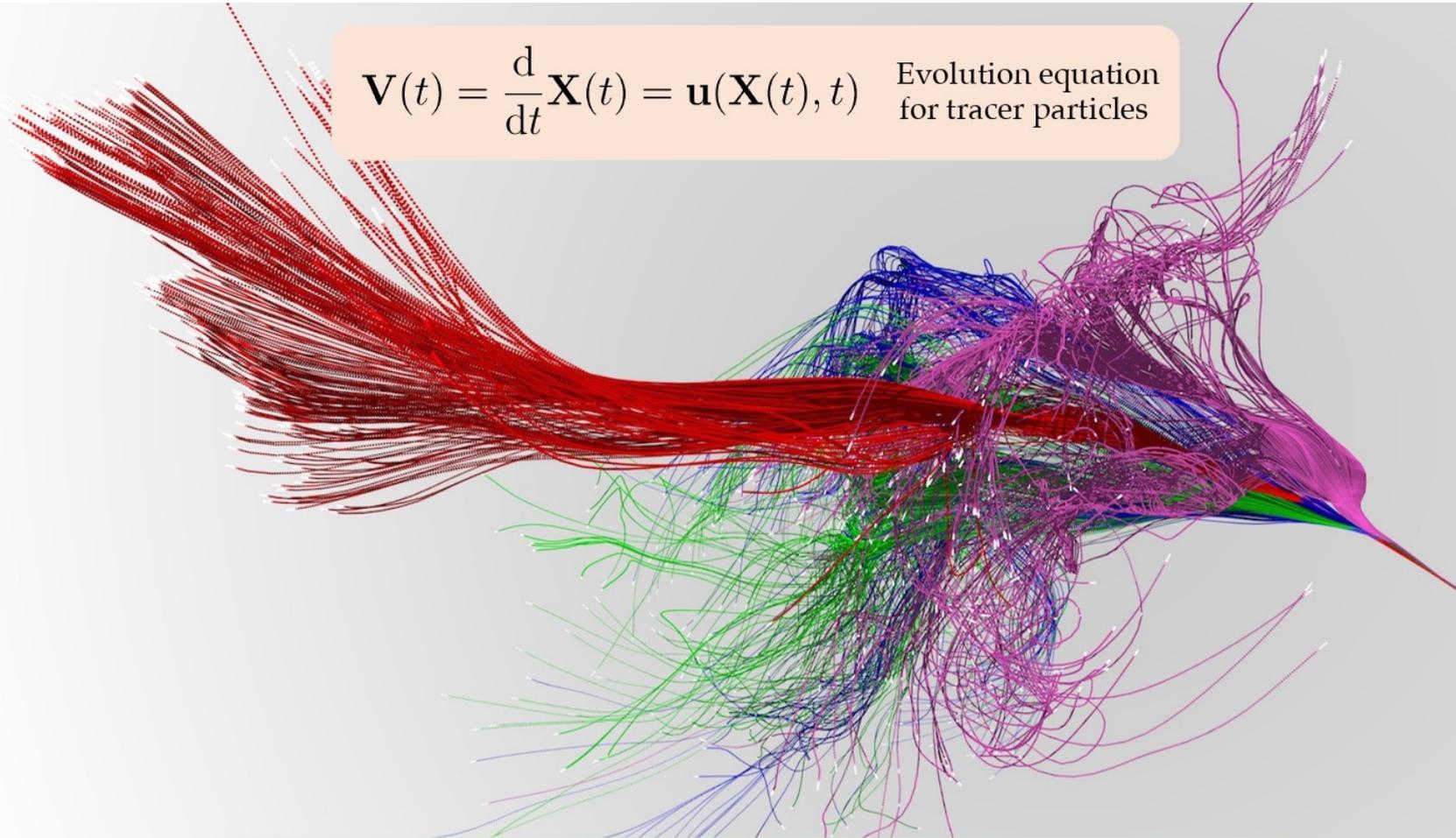
- They are not optimized
- + They need only partial information
- + They are stable wrt variation of the initial condition
- + They work also with a discrete decision time

Next step: Reinforcement Learning

- + It is optimized
- + It is model free
- + It needs partial information
- It is data-hungry

LAGRANGIAN TURBULENCE

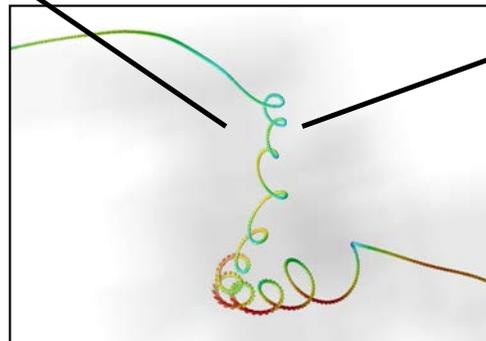
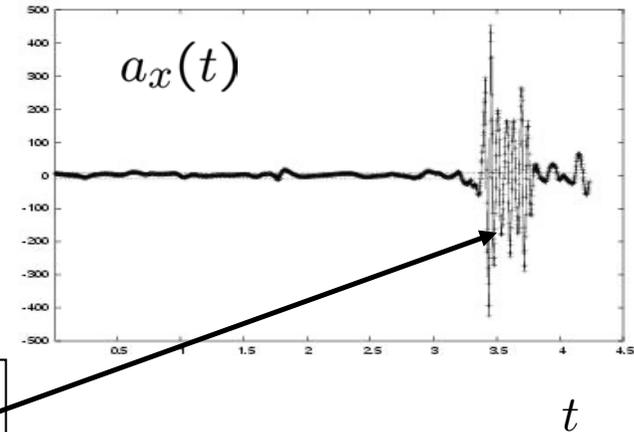
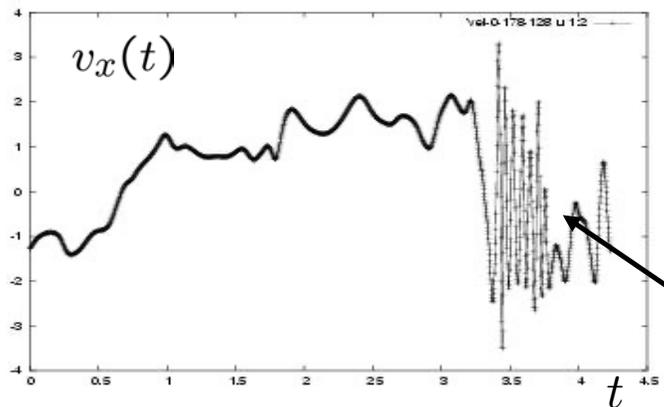
$$\mathbf{V}(t) = \frac{d}{dt} \mathbf{X}(t) = \mathbf{u}(\mathbf{X}(t), t) \quad \text{Evolution equation for tracer particles}$$



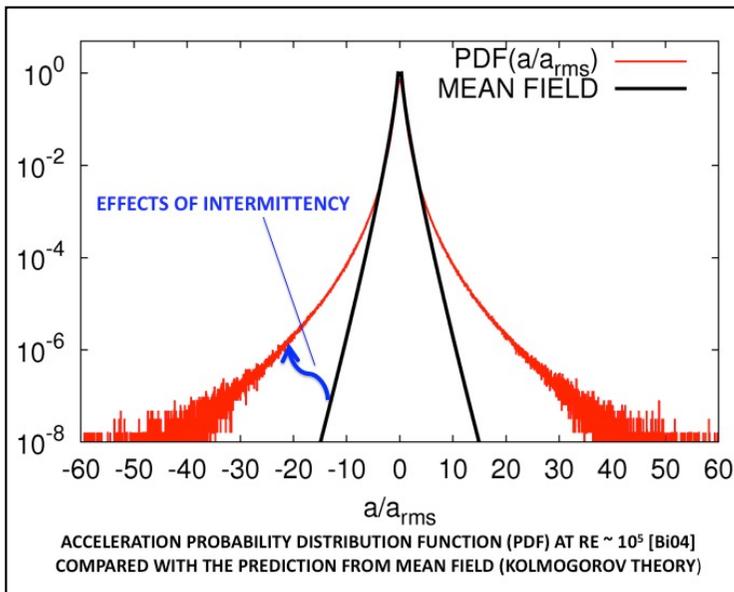
$$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \frac{1}{Re} \Delta \mathbf{u} + \mathbf{F} \\ \nabla \cdot \mathbf{u} = 0 \end{cases} \quad \begin{array}{l} \text{Navier-Stokes} \\ \text{Eq.s} \end{array}$$

Biferale et al. (J. Fluid Mech., 2014, vol. 757, pp. 550–572)

$$\begin{cases} \mathbf{a} = \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \nu \Delta \mathbf{u} + \mathbf{f} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$



EXTREME EVENTS



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La Porta, G.A. Voth, A.M. Crawford, J. Alexander et al. Fluid particle accelerations in fully developed turbulence. *Nature*, 409(6823), 1017 (2001)

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L. B., G. Boffetta, A. Celani, B. Devenish, A. Lanotte and F. Toschi. [Multifractal statistics of Lagrangian velocity and acceleration in turbulence](#). *Phys. Rev. Lett.* 93, 064502 (2004).

Generation of Lagrangian trajectories

GAN



["A Style-Based Generator Architecture for Generative Adversarial Networks" Karras, Laine & Aila, NVIDIA, 2019](#)

Diffusion Models



["Diffusion Models Beat GANs on Image Synthesis" Dhariwal & Nichol, OpenAI, 2021](#)

Diffusion Models

‘Synthetica Lagrangian Turbulence: all you need ia Diffusion Models’ T. Li, L.B, F. Bonaccorso, M. Scarpolini and M. Buzzicotti (in preparation, 2023)

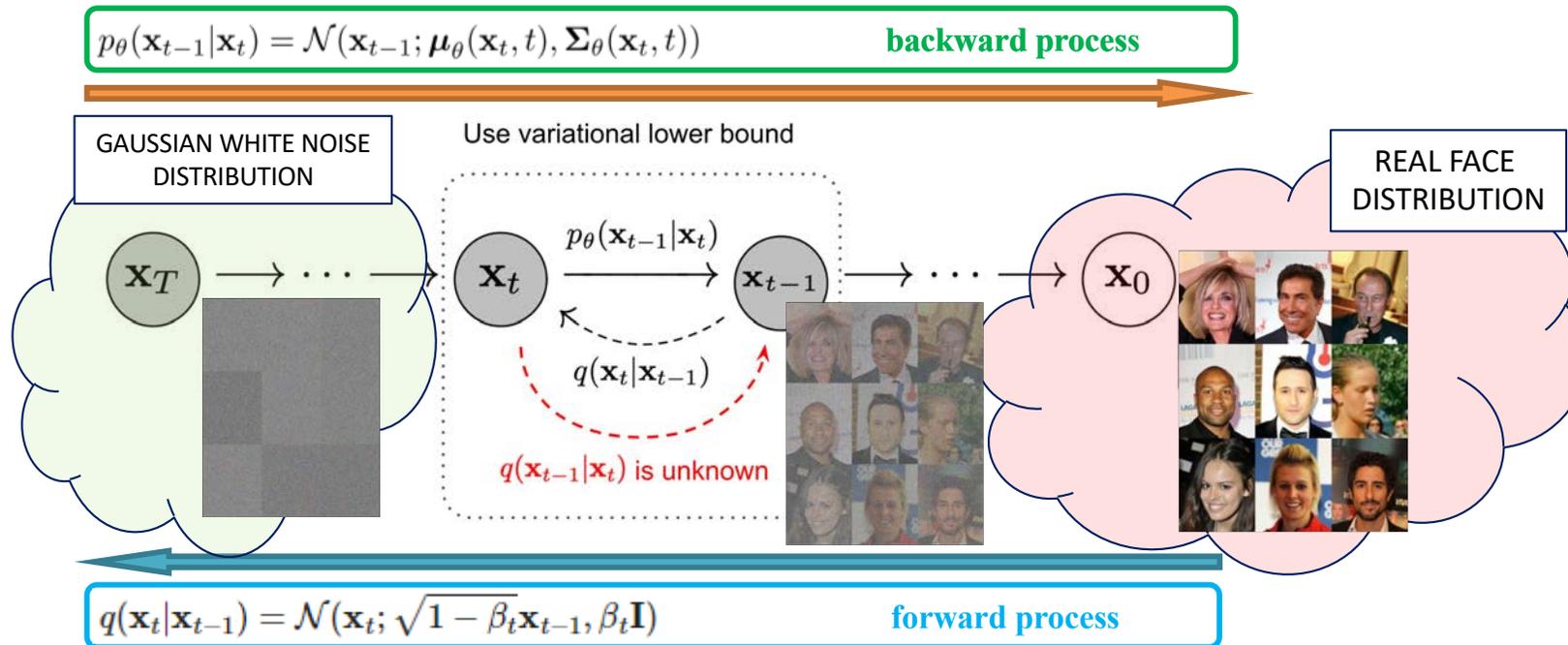
Training objective:
Maximize the likelihood

Diffusion Model

Single precision
4GPUs: => 9hrs => 20480 samples
16GPUs: => 24hrs => 204800 samples

GAN

Double precision (to be checked)
1GPU: 2s => 20480 predictions



[Sohl-Dickstein et al., Deep Unsupervised Learning using Nonequilibrium Thermodynamics, ICML 2015](#)
[Ho et al., Denoising Diffusion Probabilistic Models, NeurIPS 2020](#)
[Song et al., Score-Based Generative Modeling through Stochastic Differential Equations, ICLR 2021](#)

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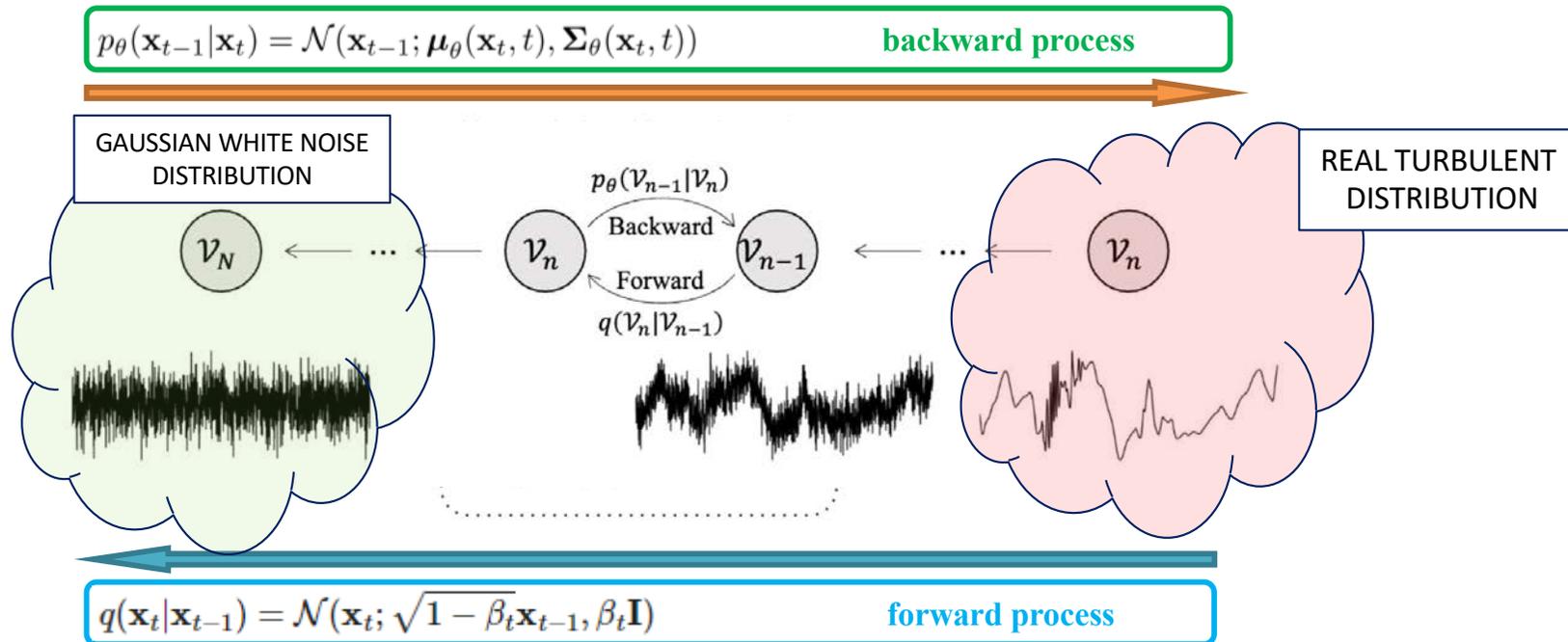
Training objective:
Maximize the likelihood

Diffusion Model

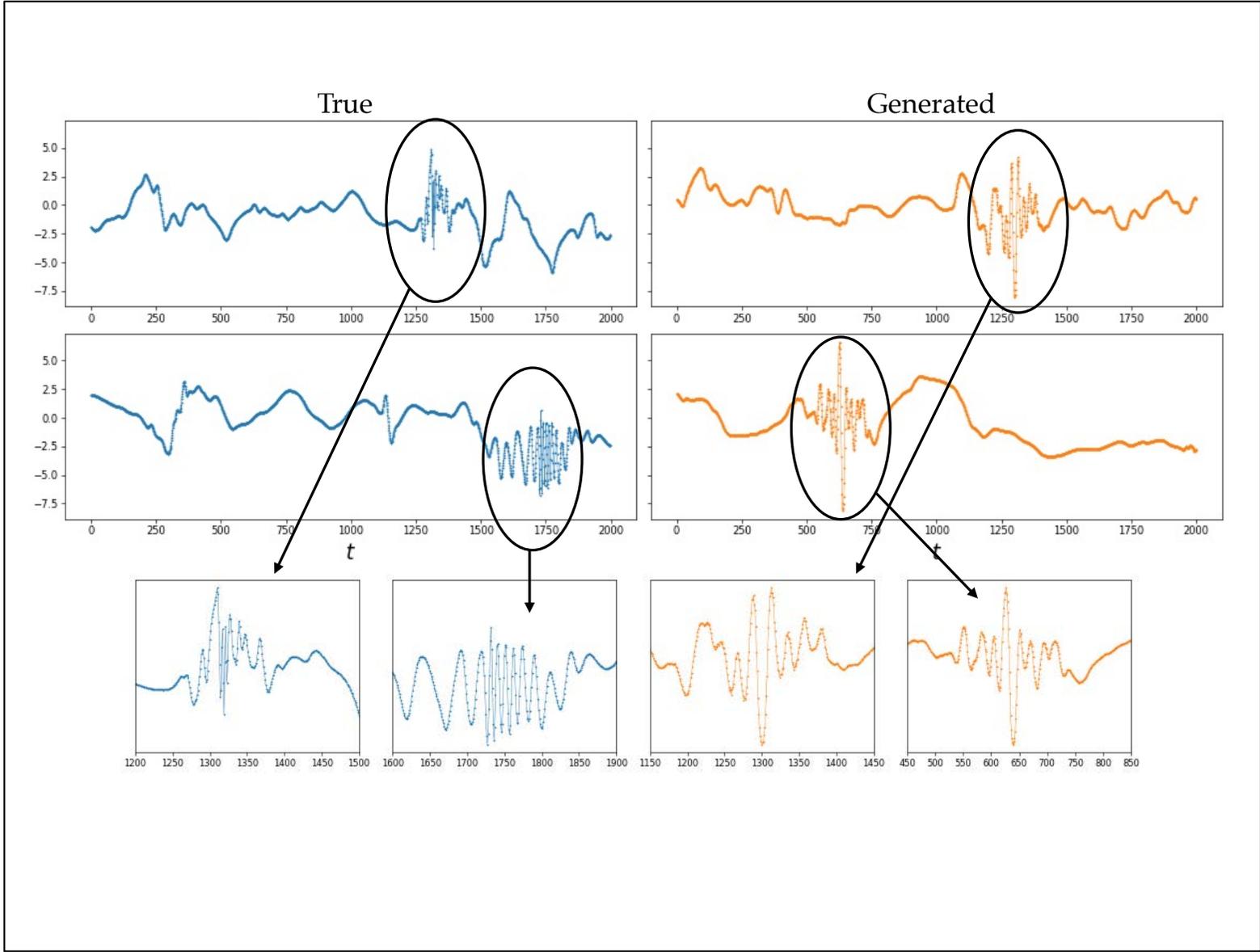
GAN

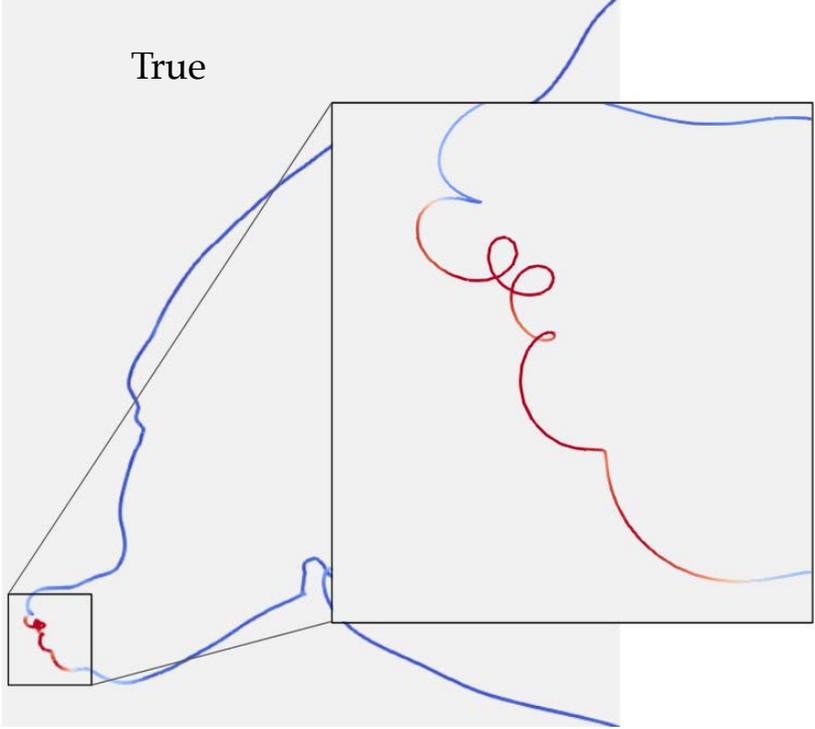
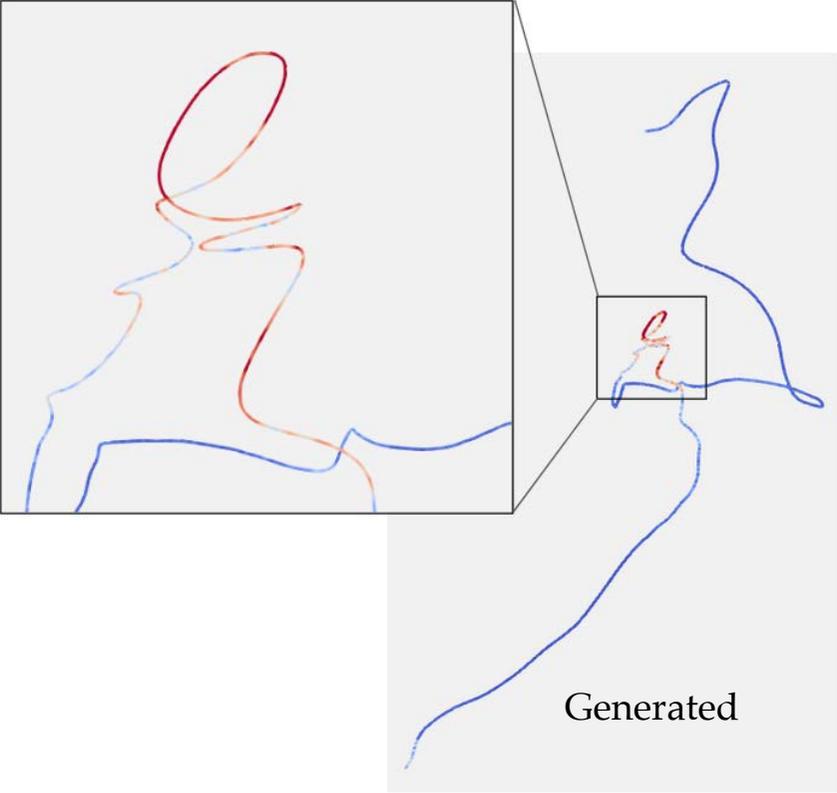
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[Song et al., Score-Based Generative Modeling through Stochastic Differential Equations, ICLR 2021](#)

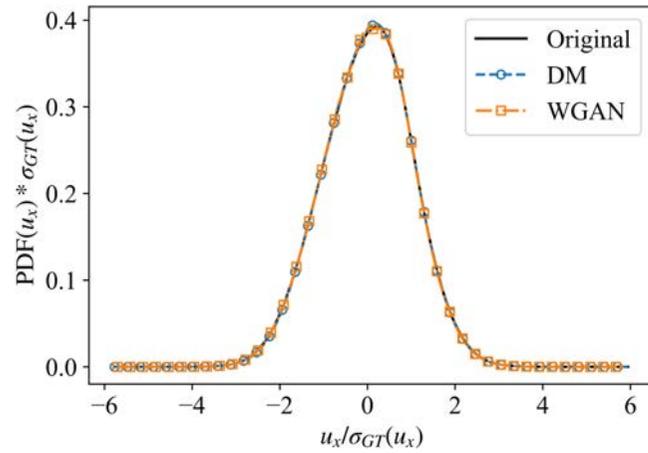




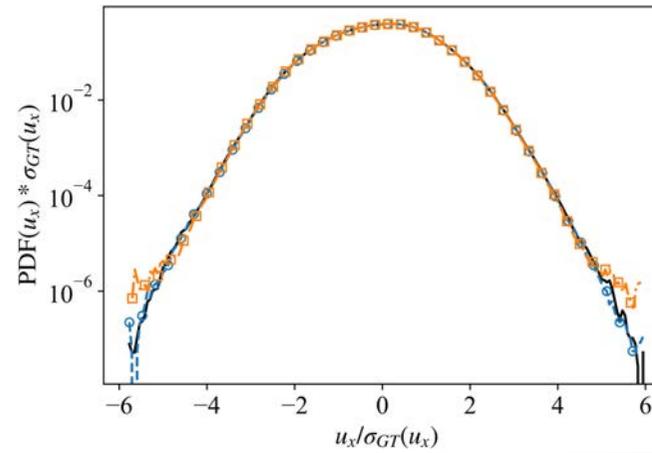
Statistics obtained from training on 327680 trajectories of length 2048 time steps (roughly 1 T_L)

PDFs are normalized with the same standard deviation of the ground truth, σ_{GT}

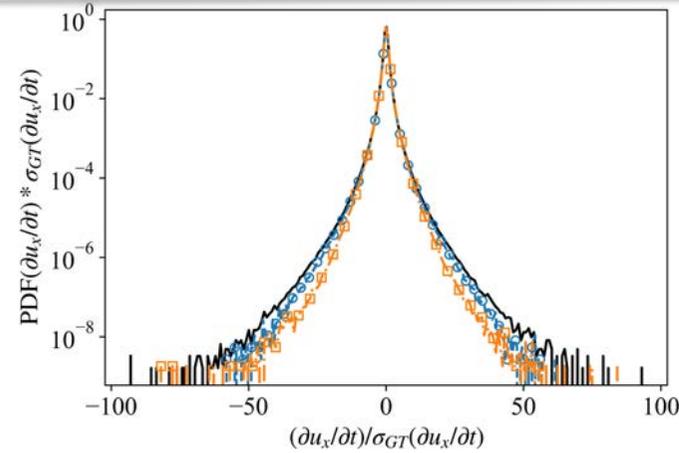
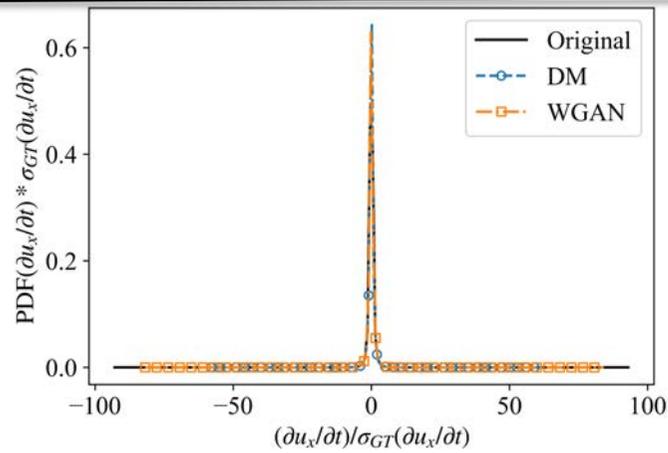
LIN-LIN PDF



LOG-LIN PDF

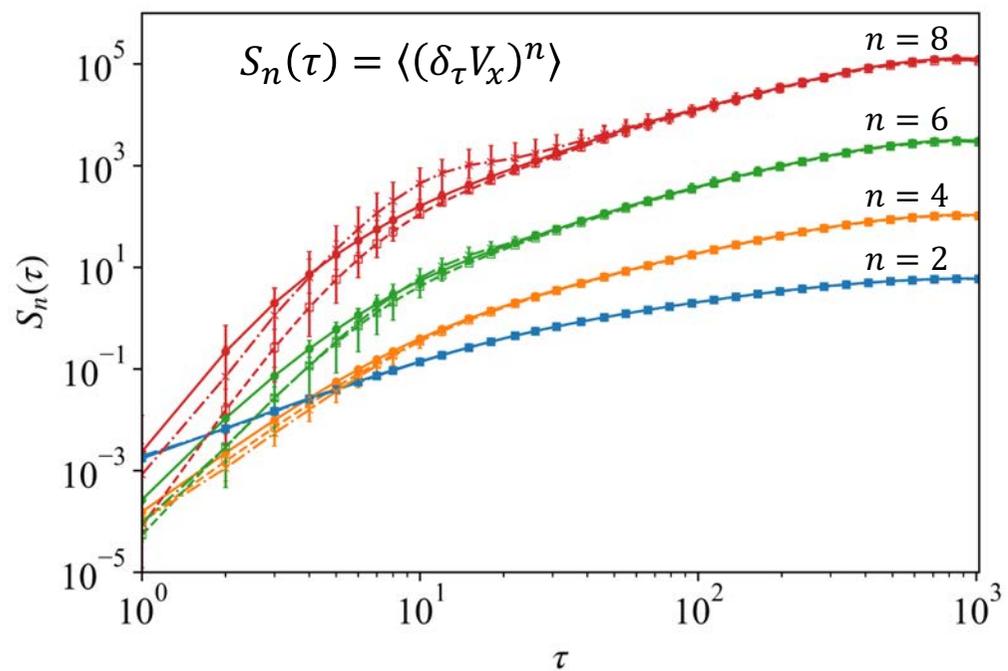


VELOCITY PDF

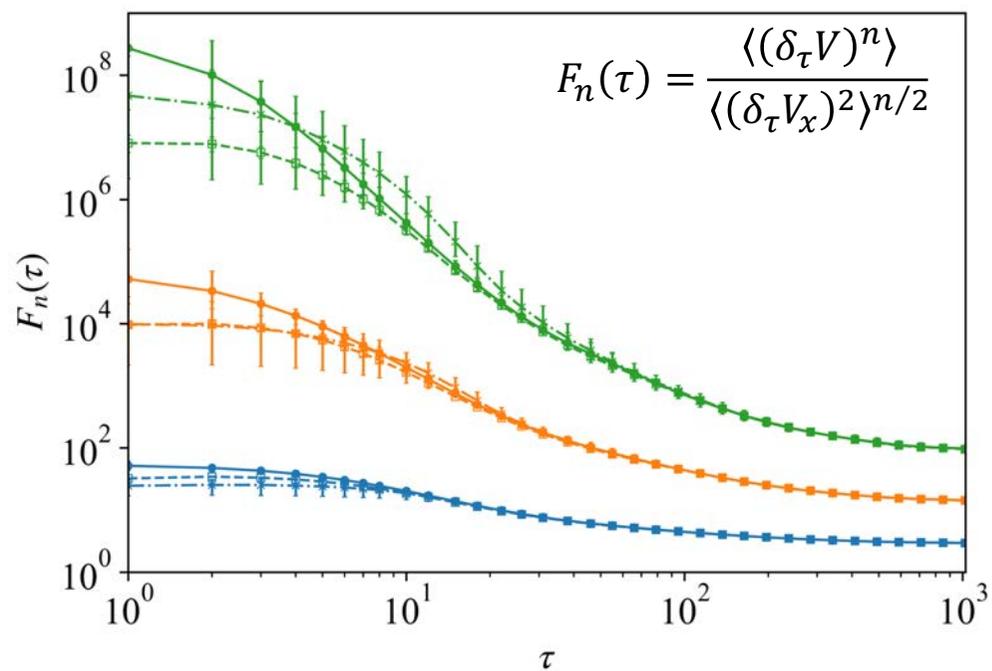


ACCELERATION PDF

LAGRANGIAN STRUCTURE FUNCTIONS



GENERALIZED FLATNESS



Original: solid circle; DM: dashed square; WGAN: dash-dotted x



Guide for users

What is *Smart-TURB*? It is a brand new software infrastructure (born June 2020) for the research community working on turbulence and complex flows with particular emphasis to collect/standardize and preserve huge datasets of big-data and Machine Learning approaches to fluid mechanics in general. In particular, it is an easily accessible web platform for high quality data that is able to host, standardize and manage a large collection of experimental and numerical data sets from high-end fluid dynamics facilities and High Performance Computational centers. Smart-TURB offers excellent performances when accessing/uploading/searching data. The research community is asked to contribute, by deploying freely downloadable, accurate and validated dataset for the sake of "reproducibility": The process of documenting procedures and archiving data so that others can fully reproduce scientific results. Please contact the administrator for infos about how to upload your dataset. We started by deploying a first dataset made of 2d and 3d turbulent configurations under the name of TURB-Rot. More will come.

<https://smart-turb.roma2.infn.it/>

TURB-ROT. A LARGE DATABASE OF 3D AND 2D SNAPSHOTS FROM TURBULENT ROTATING FLOWS

A PREPRINT

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🔍

1
Datasets

TURB-Rot
 A large database of 3d and 2d snapshots from turbulent rotating

TURB-Rot

2
Organizations

web_admin	1
web_admin group	member

ARE WE CLOSE TO AI SUPREMACY IN FLUID DYNAMICS? NO

- RATE OF PUBLICATIONS IN THE DOMAIN >> RATE OF READING/PEER REVIEWING -> DANGER OF INFLATIONARY ERA
- HUNDREDS OF PAPERS IN THE ARXIVES CITED BY HUNDREDS OF OTHER PAPERS WITHOUT CHECK ON THE RESULTS, **NOT EVEN WRONG!**
- **NEED FOR QUANTITATIVE AI:** SCALING, VALIDATION, BENCHMARKS, GENERALISATION, GRAND-CHALLENGES TO ESTABLISH BEST-PRACTISE
- NEED FOR PHYSICAL DIMENSIONALISATION: NETWORK STRUCTURE VS PHYSICAL PARAMETERS (deepness, structure, coding, # training data vs Reynolds, Rayleigh, Time-to-solution, Mach, Mass fraction etc...)
- **NEED FOR INTERDISCIPLINARY COLLABORATIONS:** APPLIED SCIENTISTS (FOR THE GOOD QUESTIONS) + AI SPECIALISTS (TO OPEN THE BOX) + NUMERICAL SCIENTISTS (FOR THE GOOD DATA)

2021-2026 AdG GRANT Smart-TURB

A Physics-Informed Machine-Learning Platform Smart Lagrangian Harness and Control of TURBulence

biferale@roma2.infn.it biferale@gmail.com

WE ARE HIRING
POST-DOCS



WE ARE HIRING
POST-DOCS



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