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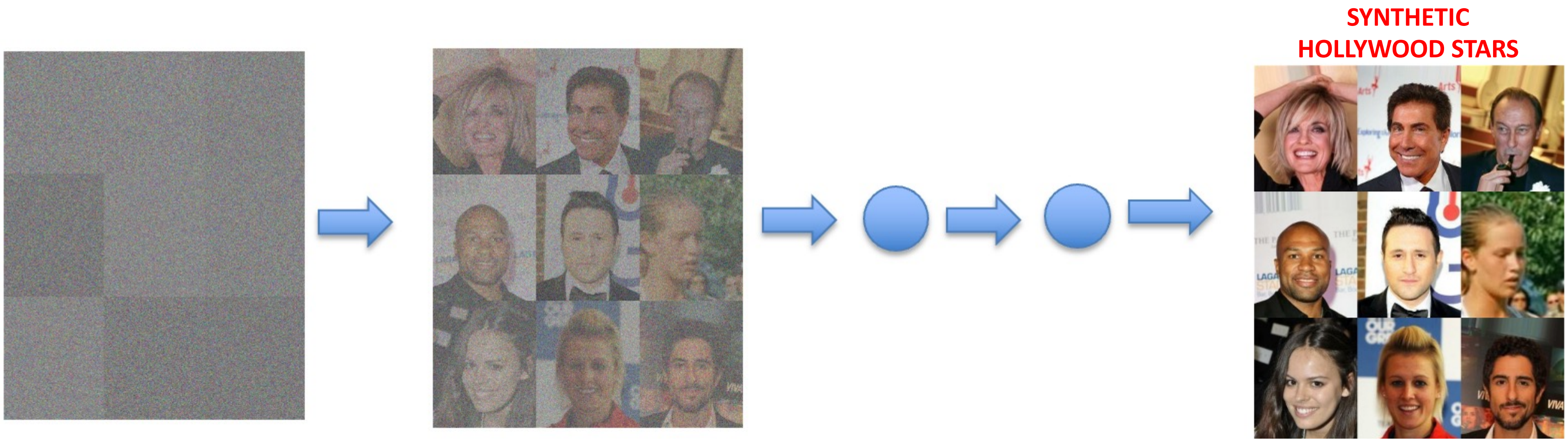

ERICE – MACHINE LEARNING FOR COMPLEXITY
2024 APRIL
Data driven tools for Eulerian and Lagrangian Turbulence

CREDITS: M. CENCINI, C. CALASCIBETTA, L. PIRO, R. HEINONEN, T. LI, F. BONACCORSO, M. BUZZICOTTI, M. SCARPOLINI

Finanziato dall'Unione europea NextGenerationEU
Ministero dell'Università e della Ricerca
Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA

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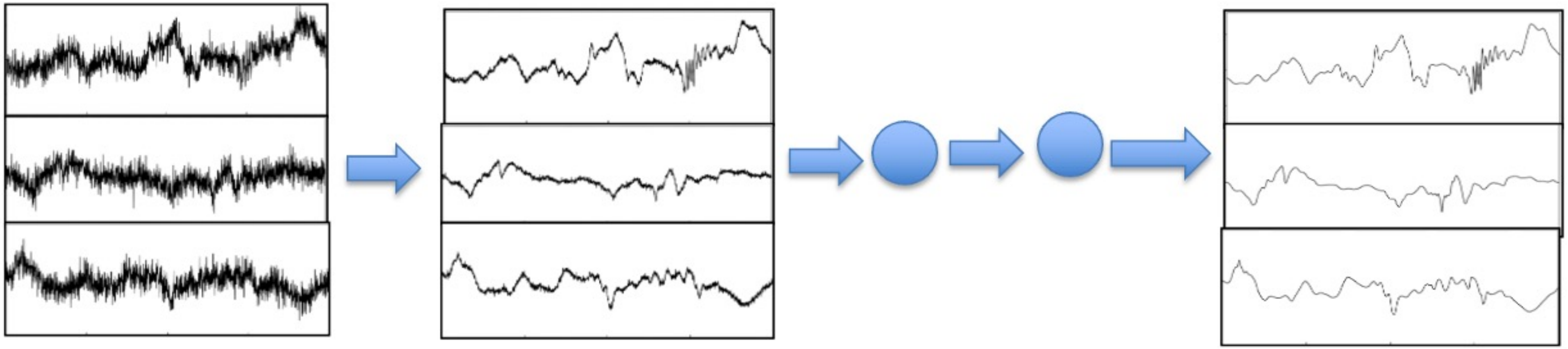
LAGRANGIAN TRAJECTORIES



CREDITS: T. LI, F. BONACCORSO, M. BUZZICOTTI, M. SCARPOLINI

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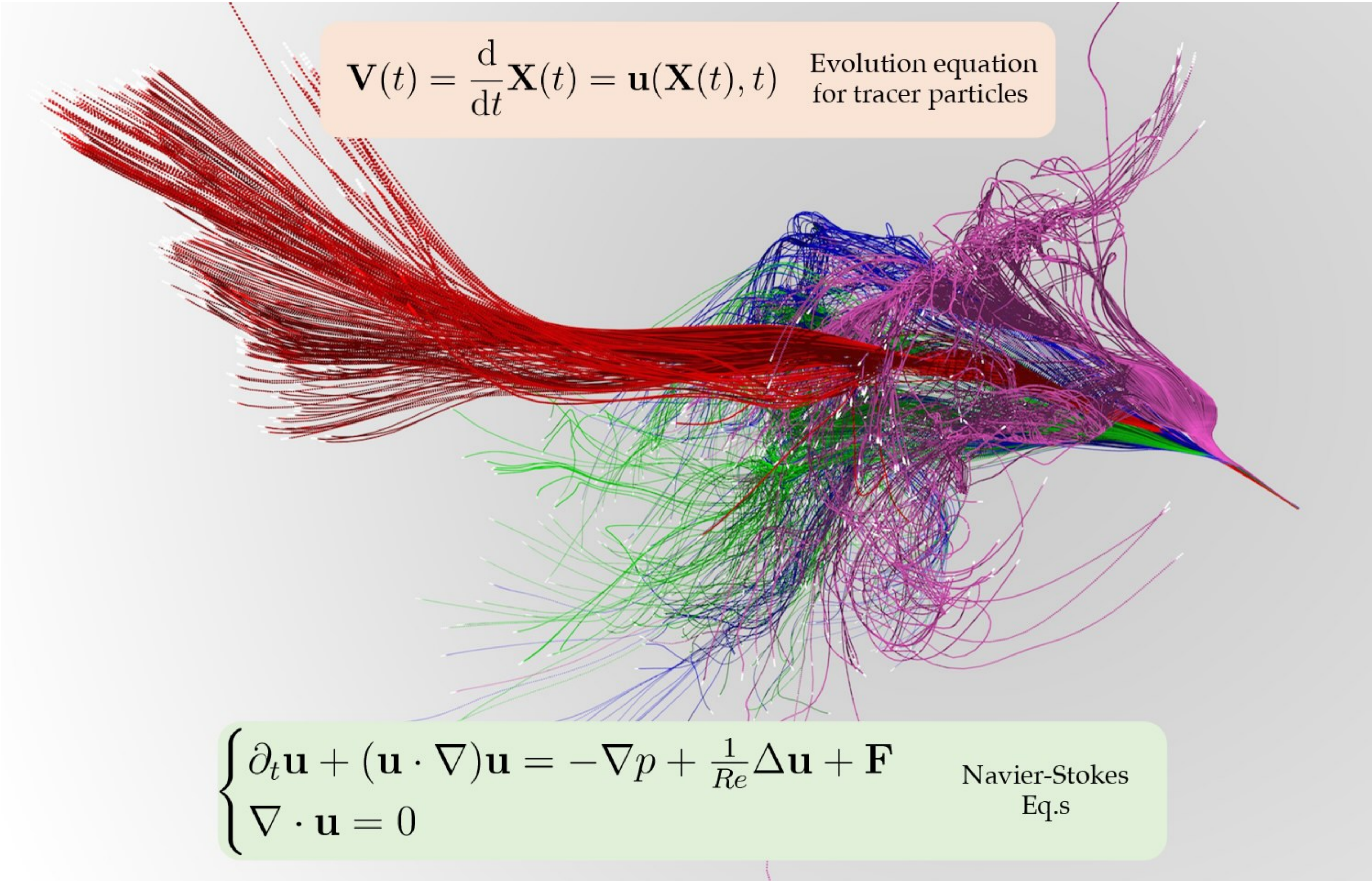


$\mathbf{V}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{X}(t) = \mathbf{u}(\mathbf{X}(t), t)$
Evolution equation for tracer particles
$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \frac{1}{Re}\Delta\mathbf{u} + \mathbf{F} \\ \nabla\cdot\mathbf{u} = 0 \end{cases}$
Navier-Stokes Eq.s

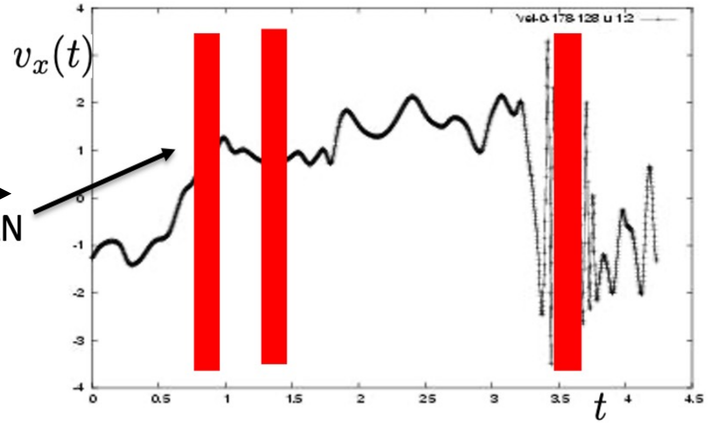
STOCHASTIC MODELS FOR LAGRANGIAN TURBULENCE: WHY?

T. Li, LB, F. Bonaccorso, M. Scarpolini, M. Buzzicotti.
Synthetic Lagrangian Turbulence by Generative Diffusion Models.
arXiv:2307.08529 (2023) – Nature Machine Intelligence APRIL 2024

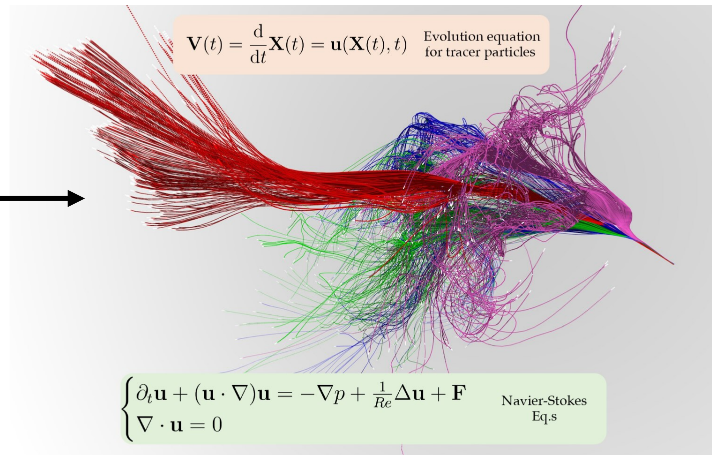
GENERATION OF LARGE SYNTHETIC DATA-BASE FOR
(I) RANKING OF PHYSICS FEATURES
(II) TESTING DOWNSTREAM APPLICATIONS/MODELS

DATA ASSIMILATION/INPAINTING FROM MISSING FIELD/EXPERIMENTAL OBERVATION

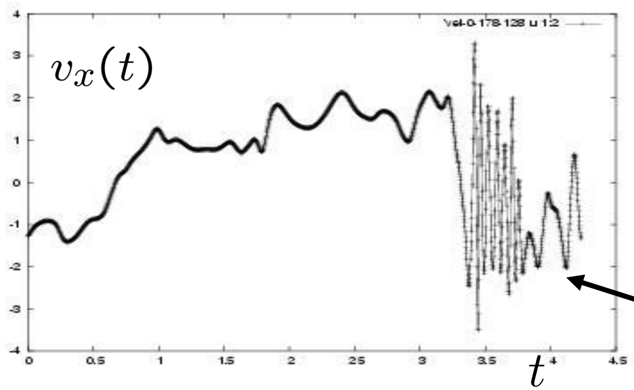
LAGRANGIAN

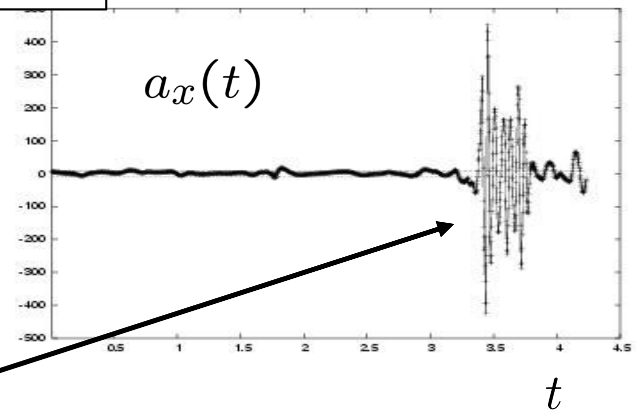


CLASSIFICATION/INFERRAL OF MISSING/INTERNAL PROPERTIES:
(I) INERTIA
(II) SHAPE
(III) ACTIVE DEGREES OF FREEDOM
(IV) ….

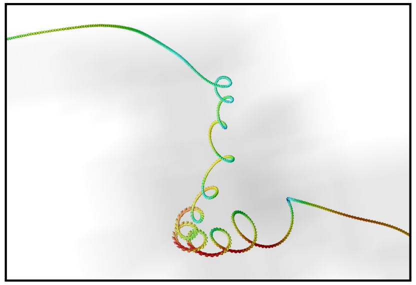


$$\begin{cases} \mathbf{a} = \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \nu \Delta \mathbf{u} + \mathbf{f} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

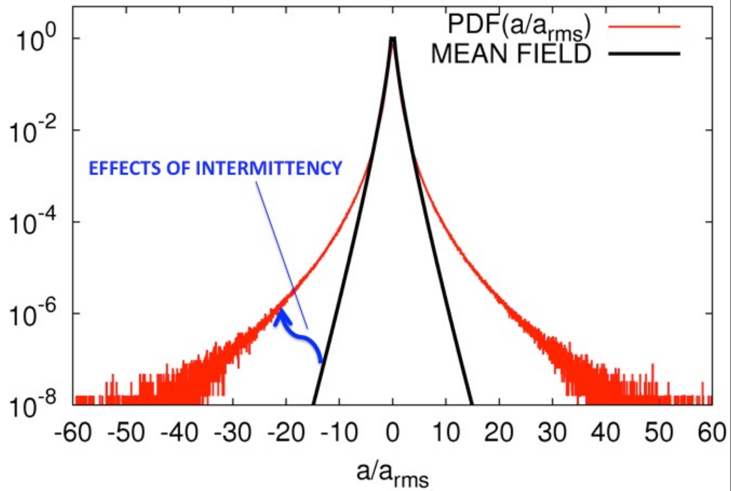




EXTREME EVENTS



$$S_i^{(p)}(\tau) = \langle [v_i(t+\tau) - v_i(t)]^p \rangle$$

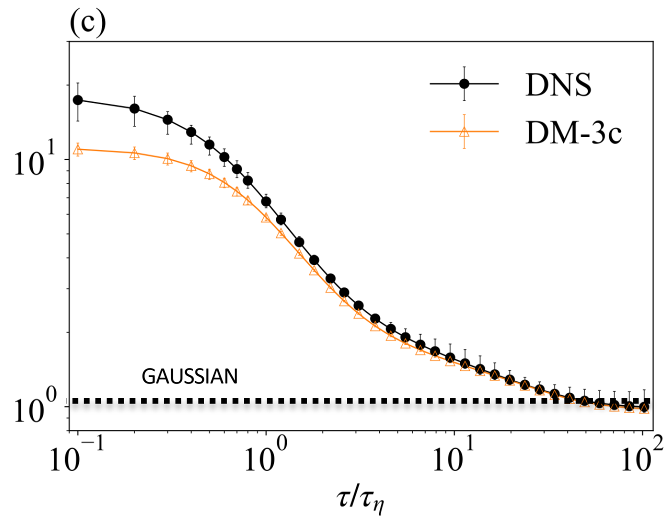


ACCELERATION PROBABILITY DISTRIBUTION FUNCTION (PDF) AT RE ~ 10^5 [Bi04] COMPARED WITH THE PREDICTION FROM MEAN FIELD (KOLMOGOROV THEORY)

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

N. Mordant, P. Metz, O. Michel and J.F. Pinton. Measurement of Lagrangian velocity in fully developed turbulence. Phys. Rev. Lett. 87(21), 214501 (2001)

F. Toschi and E. Bodenschatz. Lagrangian Properties of Particles in Turbulence. Annu. Rev. Fluid Mech. 41, 375 (2009)



$$F(\tau) = \frac{S^{(4)}(\tau)}{[S^{(2)}(\tau)]^2}$$

$$S_i^{(p)}(\tau) = \langle [v_i(t+\tau) - v_i(t)]^p \rangle$$

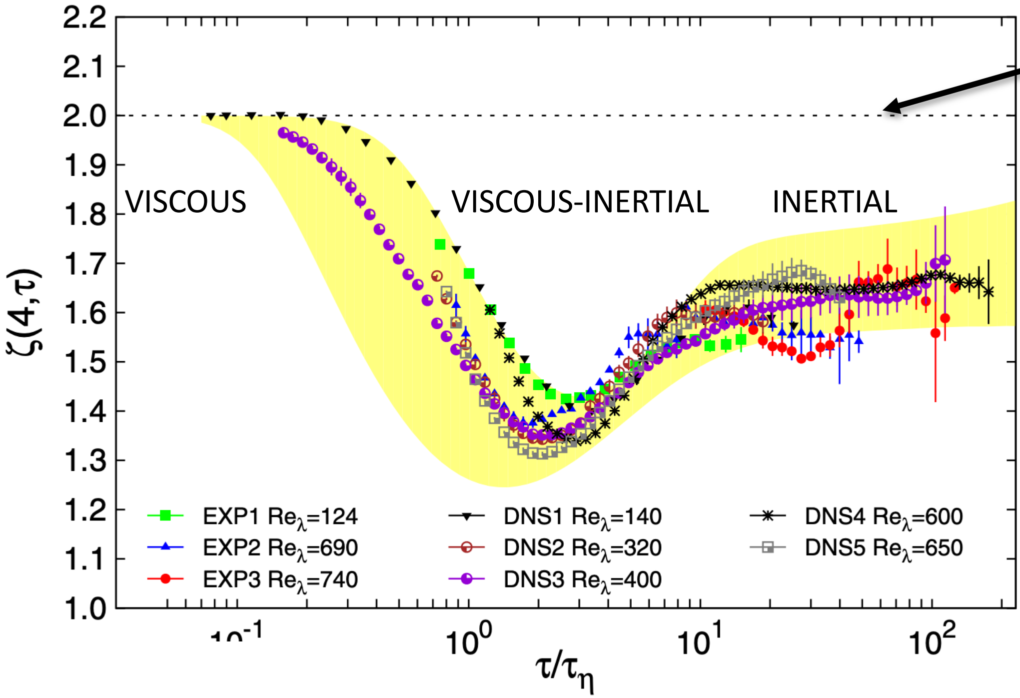
$$\zeta(4,\tau) = \frac{d \log S^{(4)}(\tau)}{d \log S^{(2)}(\tau)}$$

PRL 100, 254504 (2008) PHYSICAL REVIEW LETTERS week ending 27 JUNE 2008

Universal Intermittent Properties of Particle Trajectories in Highly Turbulent Flows

A. Arnèodo,[1] R. Benzi,[2] J. Berg,[3] L. Biferale,[4,*] E. Bodenschatz,[5] A. Busse,[6] E. Calzavarini,[7] B. Castaing,[1] M. Cencini,[8,*] L. Chevillard,[1] R. T. Fisher,[9] R. Grauer,[10] H. Homann,[10] D. Lamb,[9] A. S. Lanotte,[11,*] E. Lévèque,[1] B. Lüthi,[12] J. Mann,[3] N. Mordant,[13] W.-C. Müller,[6] S. Ott,[3] N. T. Ouellette,[14] J.-F. Pinton,[1] S. B. Pope,[15] S. G. Roux,[1] F. Toschi,[16,17,*] H. Xu,[5] and P. K. Yeung[18]

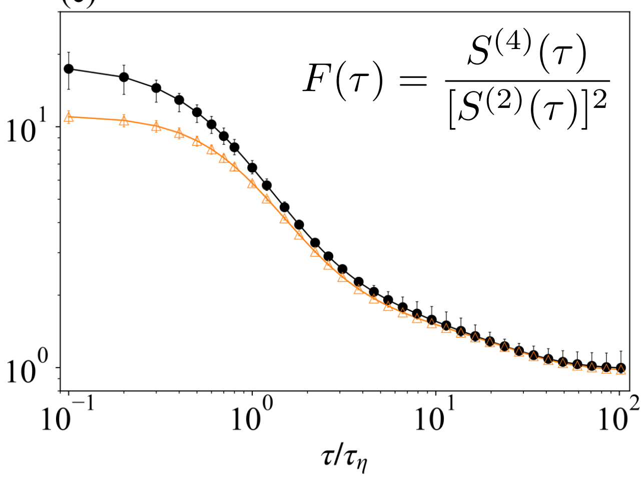
(International Collaboration for Turbulence Research)



GAUSSIAN – NO INTERMITTENCY

- UNIVERSALITY
- SCALE-BY-SCALE INTERMITTENCY
- VISCOUS-SCALE FLUCTUATIONS
- MF-PREDICTION

(c)



M. Borgas “The multifractal Lagrangian nature of turbulence”, PTRSA 342, 379 (1993)
G. K. Batchelor. “Pressure fluctuations in isotropic turbulence” Proc. Camb. Philos. Soc. 47, 359 (1951)
G. Paladin and A. Vulpiani, “Degrees of freedom of turbulence,” Phys. Rev. A 35, 1971 (1987)
C. Meneveau, “Transition between viscous and inertial-range scaling of turbulence structure functions“ Phys. Rev. E 54, 3657 (1996)

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Arnéodo, A. et al. Universal intermittent properties of particle trajectories in highly turbulent flows. Physical Review Letters 100, 254504 (2008

Pope, S. B. Simple models of turbulent flows. Physics of Fluids 23, 011301 (2011).

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particle simulations of single-phase and dispersed two-phase turbulent flows. Physics of Fluids 26, 113303 (2014).

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probabilistic representation of kolmogorov's views on turbulence. In Annales Henri Poincaré, vol. 20, 3693–3741 (Springer, 2019).

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differentiable stochastic processes. Journal of Fluid Mechanics 900, A27 (2020).

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and its synthesis in Fourier and wavelet space. J. Phys. Complex. 4 015005 (2023)

Diffusion Models

Training set: a set of images $\vec{a}^\mu \in \mathbb{R}^N$ $\mu = 1, ..., P$
N is the dimension of the data, P their number

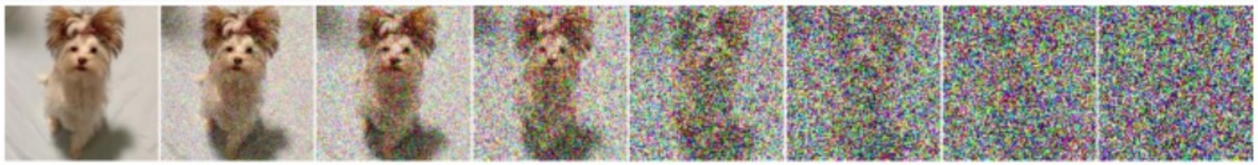
Langevin equation for an Ornstein-Uhlenbeck process

$$\frac{d\vec{x}}{dt} = -\vec{x} + \vec{\eta}(t) \qquad \langle \eta_i(t)\eta_j(t')\rangle = 2T\delta_{ij}\delta(t-t')$$

$\vec{x}^\mu(t = 0) = \vec{a}^\mu$ It transforms the data in iid Gaussian $\mathcal{N}(0,1)$ at t>>1

$$P_t(\vec{x}) = \int d\vec{a}\; P_0(\vec{a}) \frac{1}{\sqrt{2\pi\Delta_t}^N} \exp\left(-\frac{1}{2}\frac{(\vec{x}-\vec{a}e^{-t})^2}{\Delta_t}\right) = \int d\vec{a}\; P_t(\vec{a},\vec{x})$$

$$\Delta_t = T(1-e^{-2t})$$

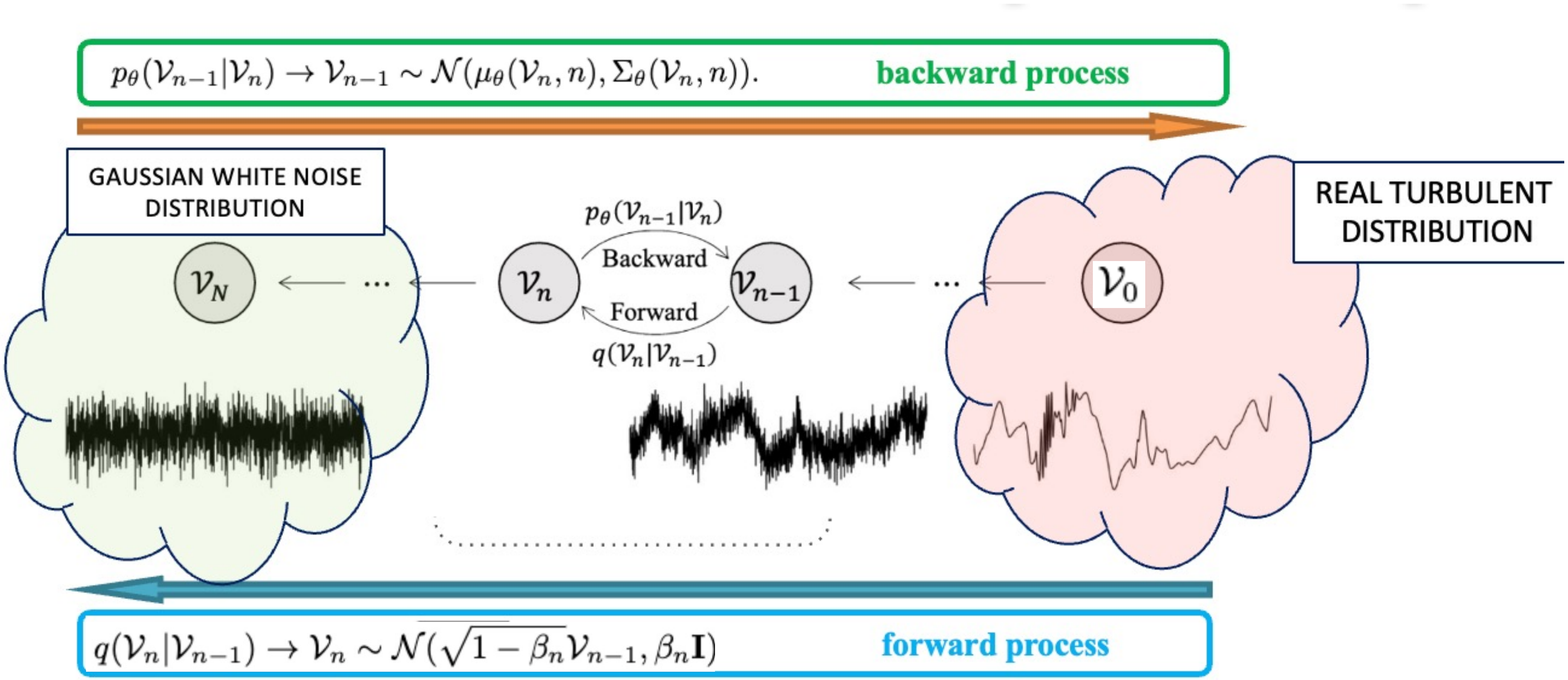


Score function provides the force field to go back in time

$$\mathcal{F}_i(\vec{x},t) = \frac{\partial \log P_t(\vec{x})}{\partial x_i} \qquad -\frac{dy_i}{dt} = y_i + 2T\mathcal{F}_i(y,t) + \eta_i(t)$$

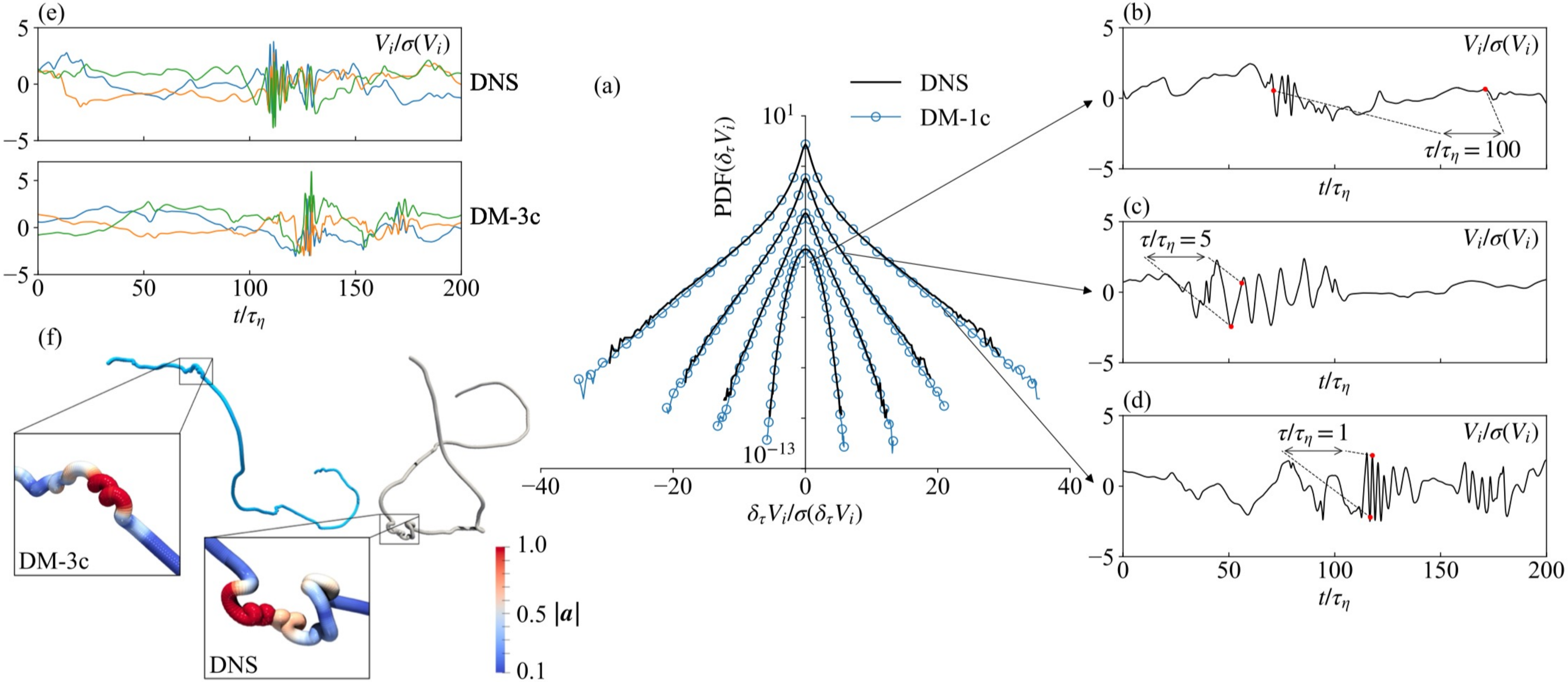
Diffusion Models

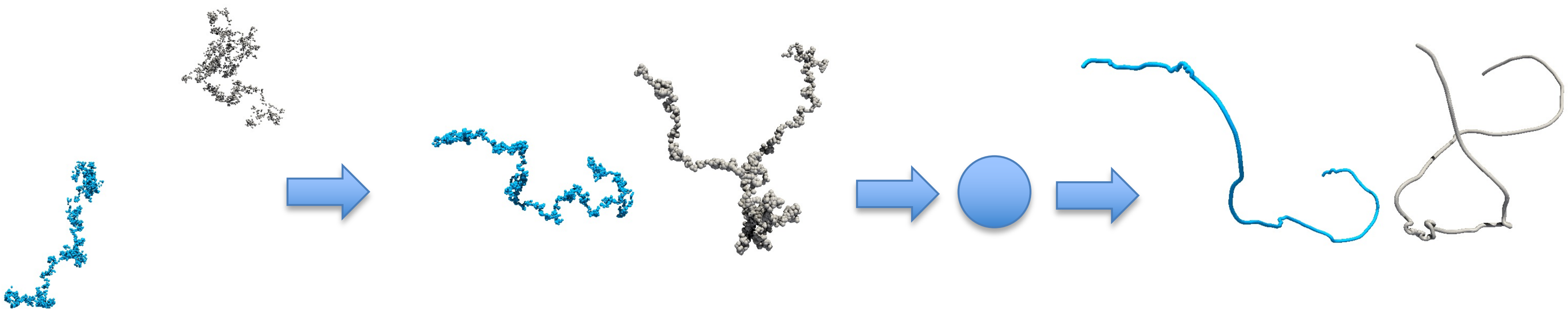
'Synthetica Lagrangian Turbulence: all you need is Diffusion Models' T. Li, L.B, F. Bonaccorso, M. Scarpolini and M. Buzzicotti (arXiv:2307.08529 2023, submitted Nature Machine Intelligence)



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

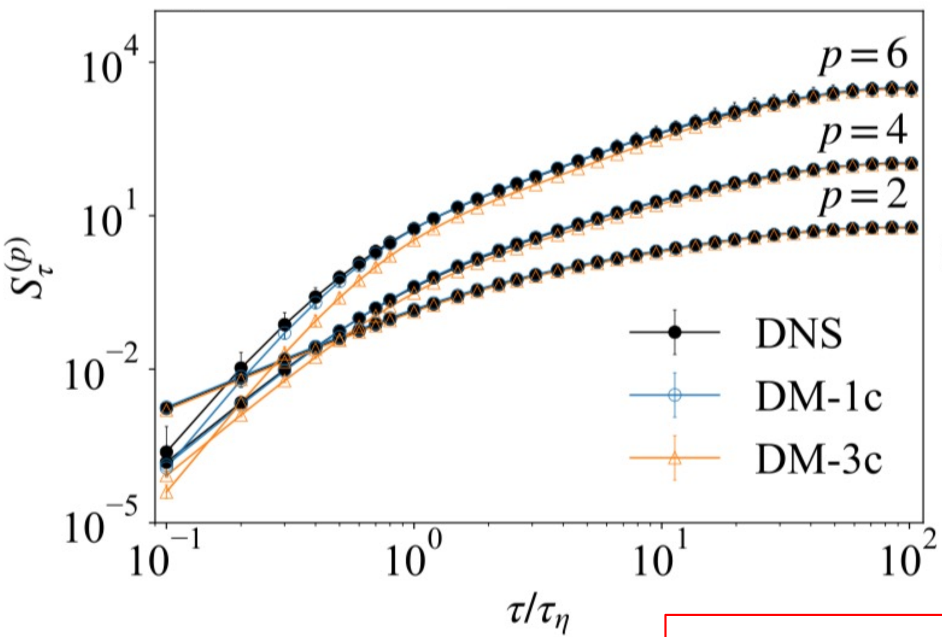
$$\delta_\tau V_i(t) = V_i(t+\tau) - V_i(t),$$





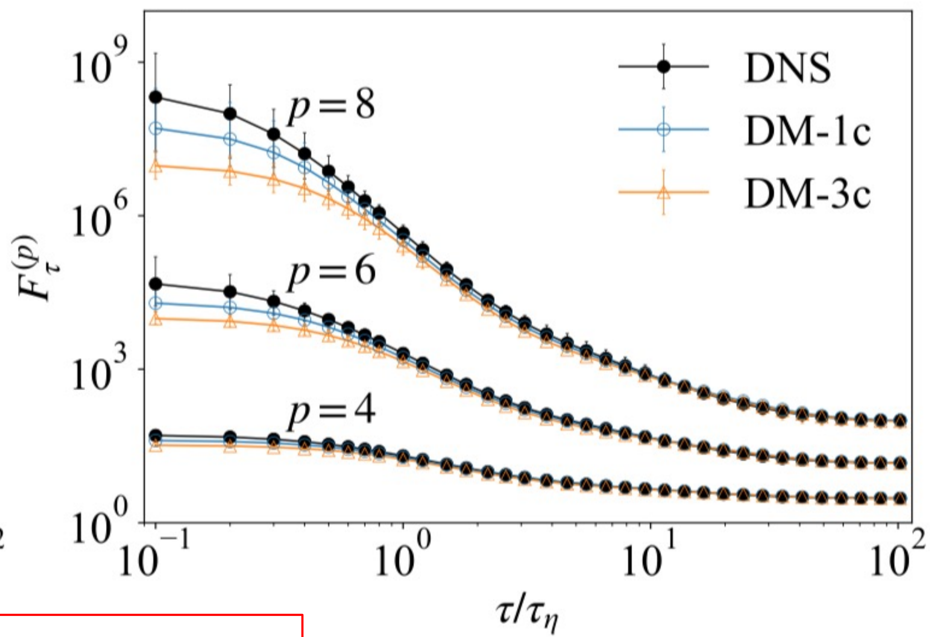
LAGRANGIAN STRUCTURE FUNCTIONS

$$S_\tau^{(p)} = \langle (\delta_\tau V_i)^p \rangle$$

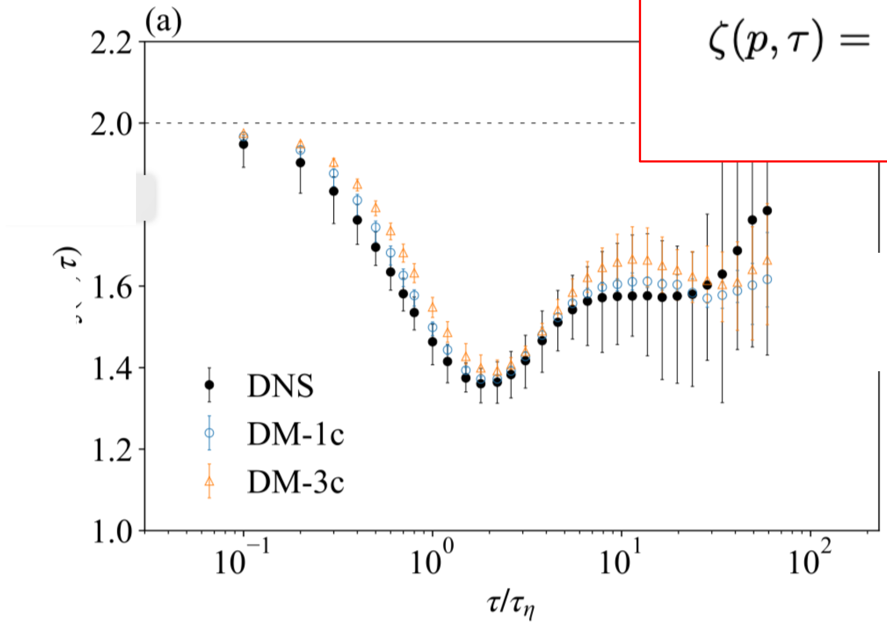


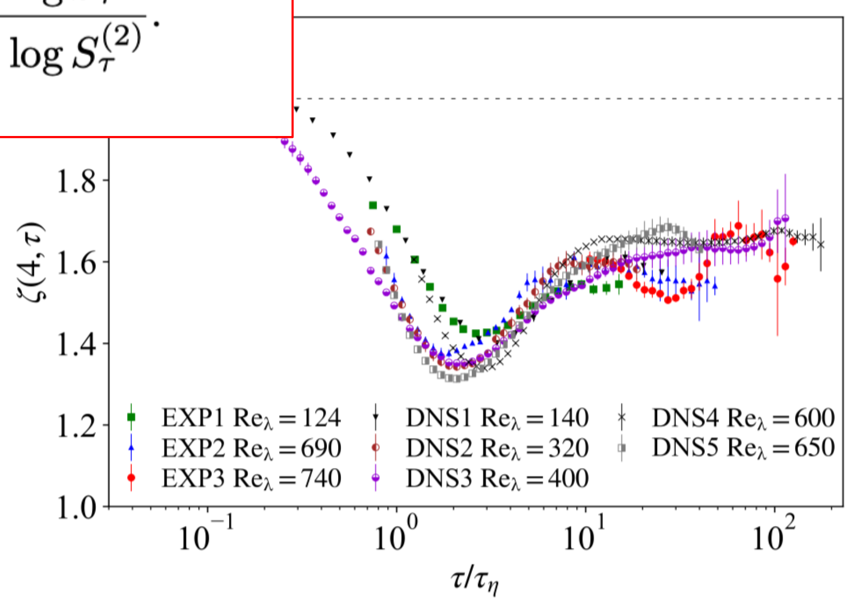
GENERALIZED FLATNESS

$$F_\tau^{(p)} = S_\tau^{(p)} / [S_\tau^{(2)}]^{p/2}.$$

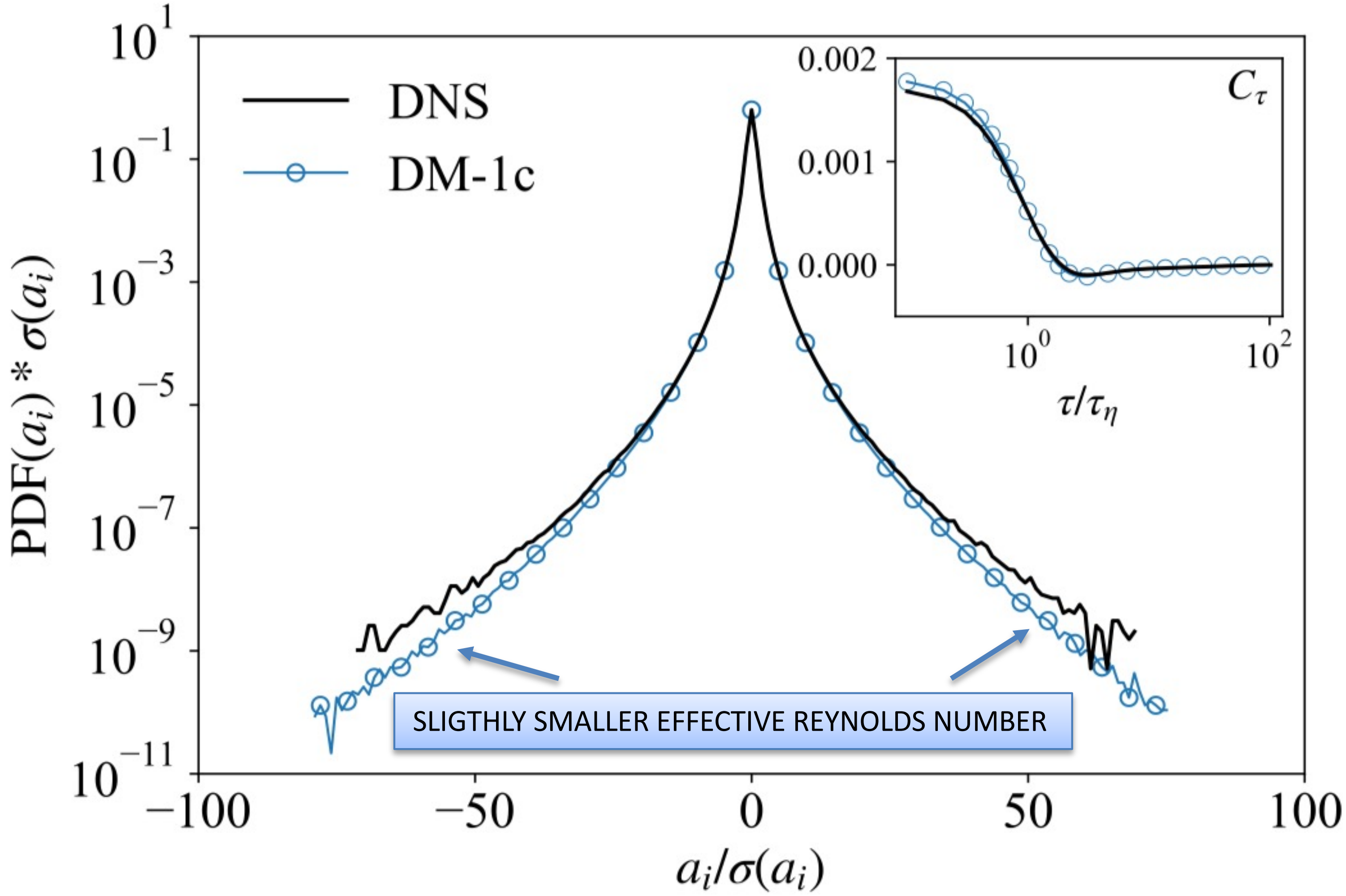


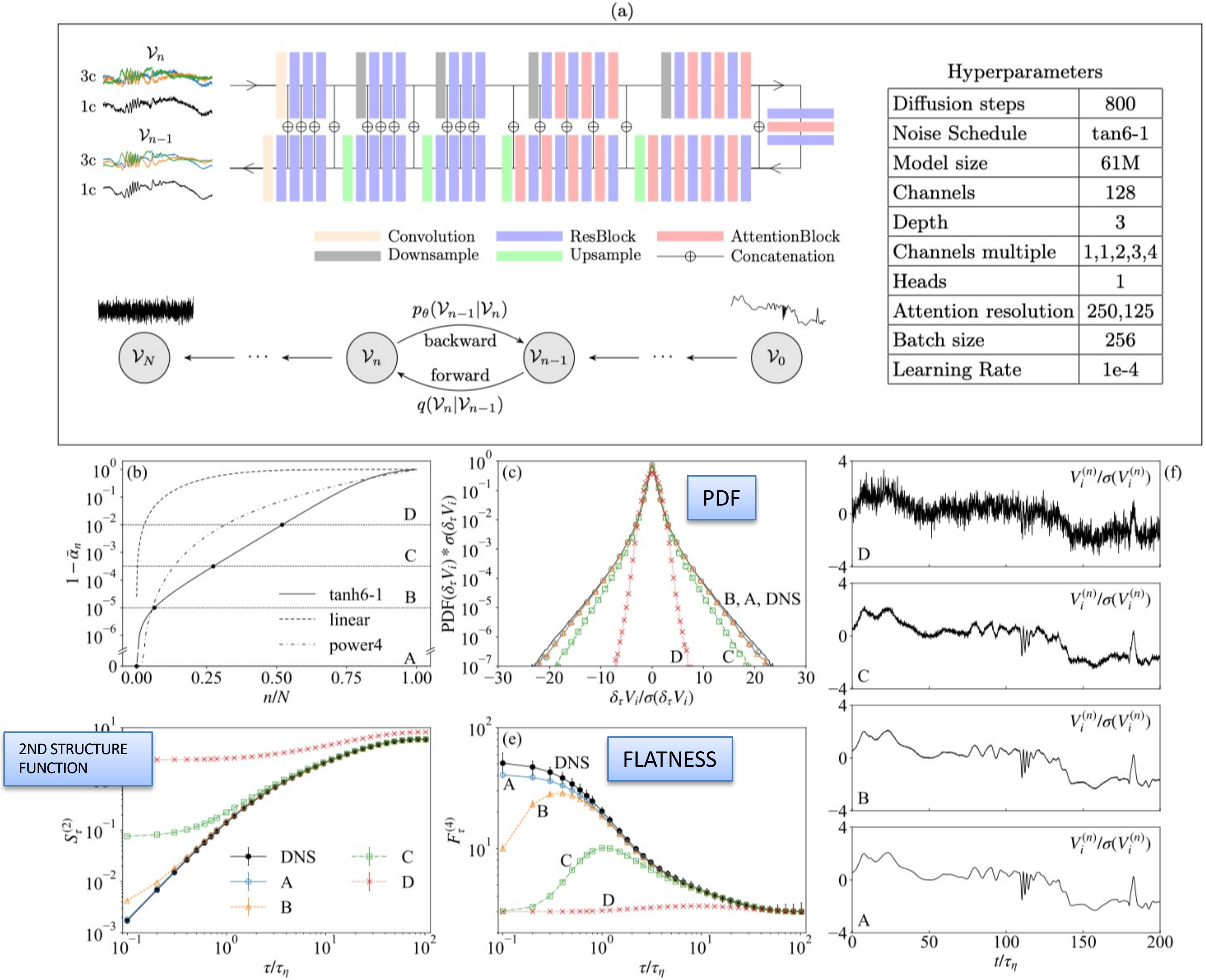
$$\zeta(p, \tau) = \frac{d \log S_\tau^{(p)}}{d \log S_\tau^{(2)}}.$$





ACCELERATION PDF





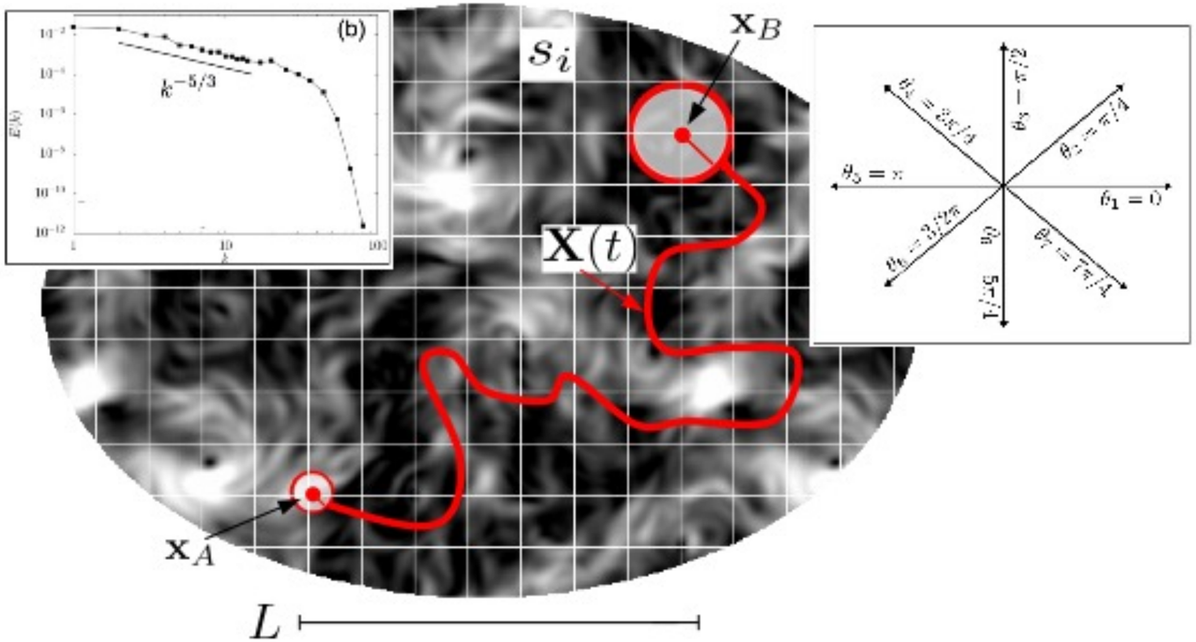
Hyperparameters

Diffusion steps	800
Noise Schedule	tan6-1
Model size	61M
Channels	128
Depth	3
Channels multiple	1,1,2,3,4
Heads	1
Attention resolution	250,125
Batch size	256
Learning Rate	1e-4

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

L. Biferale,[1] F. Bonaccorso,[1,2] M. Buzzicotti,[1] P. Clark Di Leoni,[1,3] and K. Gustavsson[4]

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



$$\begin{cases} \dot{\boldsymbol{X}}_t = \boldsymbol{u}(\boldsymbol{X}_t) + \boldsymbol{U}^{ctrl}(\boldsymbol{X}_t) \\ \boldsymbol{U}^{ctrl}(\boldsymbol{X}_t) = V_{\mathrm{s}}\boldsymbol{n}(\boldsymbol{X}_t) \end{cases}$$

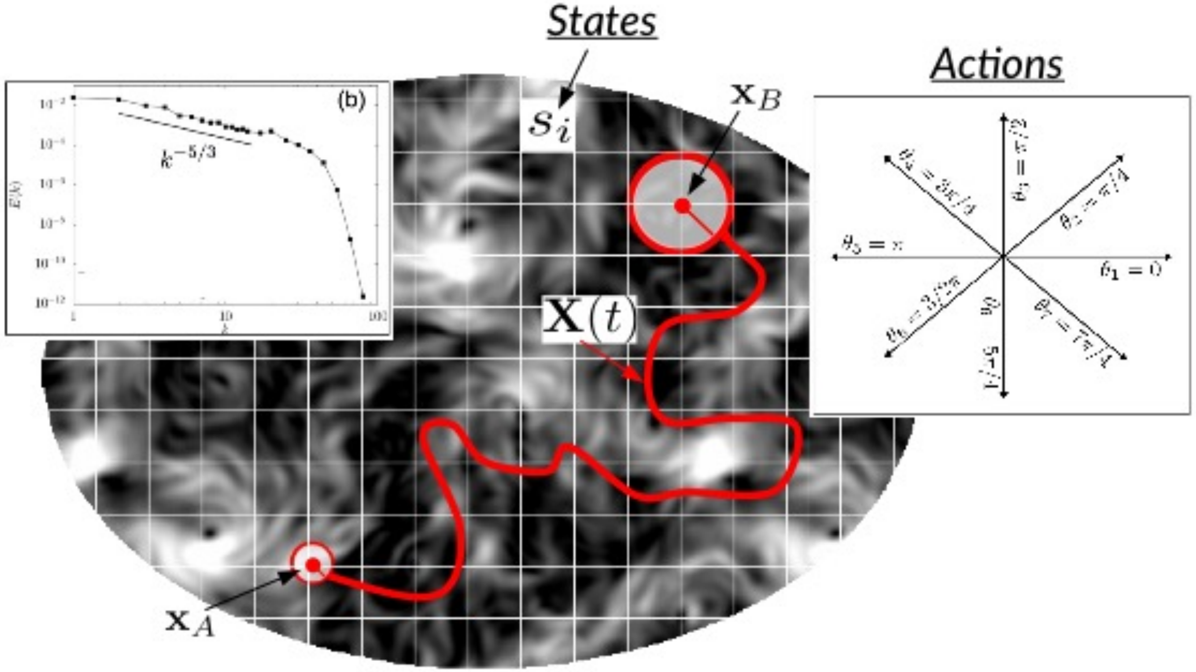
$$\boxed{\boldsymbol{n}(\boldsymbol{X}_t) = (\cos[\theta_t], \sin[\theta_t])\,,}$$

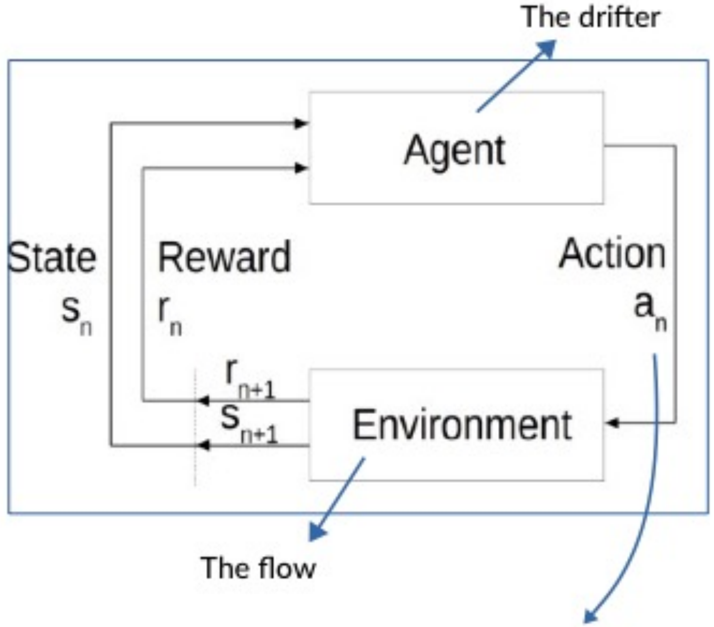
V_s → <u>Navigation speed is small compared to the velocity of the underling flow!</u>

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:

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

Parameterized state value function:

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

Reward

$$r_t = -\Delta t$$

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

Actor-Critic algorithm

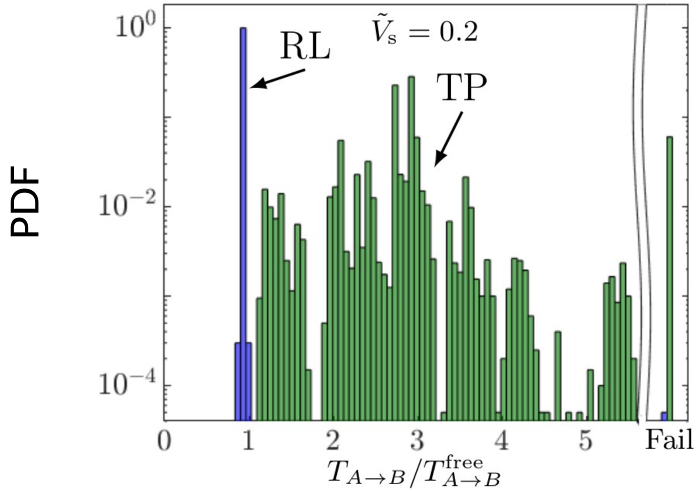
$$\begin{cases}\boldsymbol{q}_{t+\Delta t} = \boldsymbol{q}_t + \alpha_t\beta_t\nabla_{\boldsymbol{q}}\ln(\pi(a_t|s_t,\boldsymbol{q}_t))\\ \boldsymbol{w}_{t+\Delta t} = \boldsymbol{w}_t + \alpha'_t\beta_t\nabla_{\boldsymbol{w}}\hat{v}(s_t,\boldsymbol{w}_t)\end{cases}$$

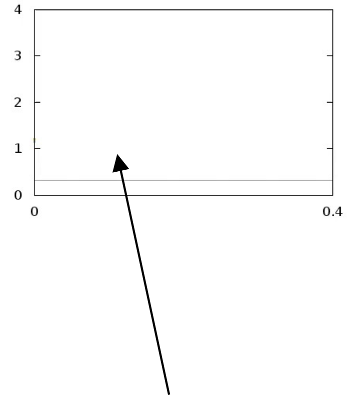
$$\beta_t = [\hat{r}_{t+\Delta_t} - \hat{v}(s_t,\boldsymbol{w}_t)] \to \text{ baseline}$$

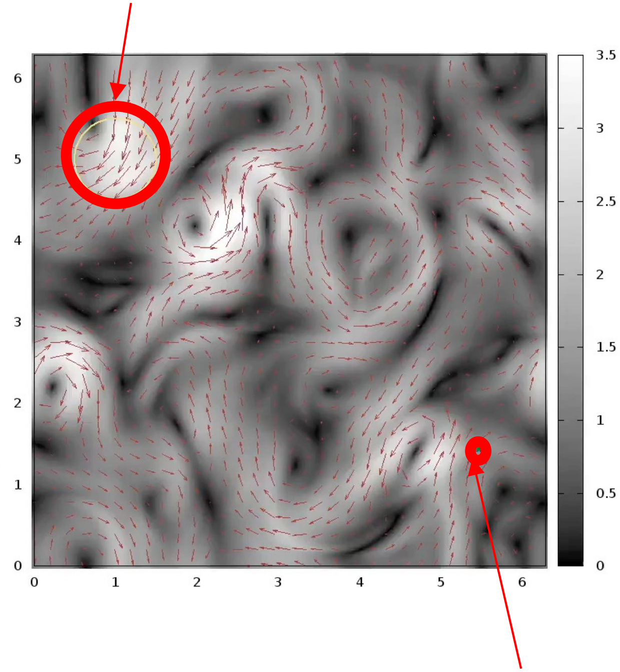
TIME-DEPENDENT 2D TURBULENT FLOWS

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

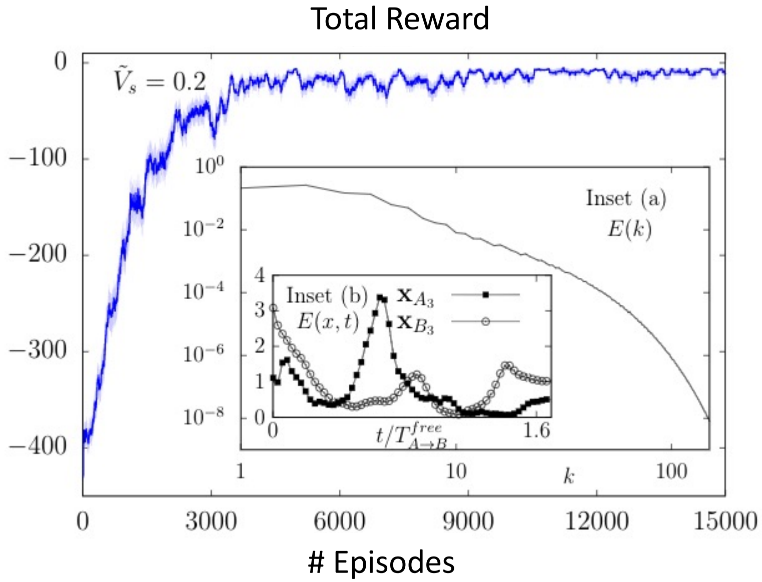
Comparison with a Trivial Policy (TP)

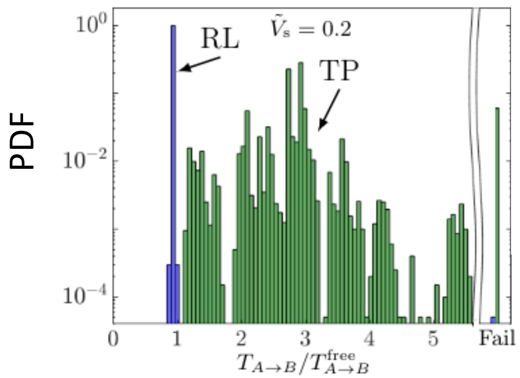


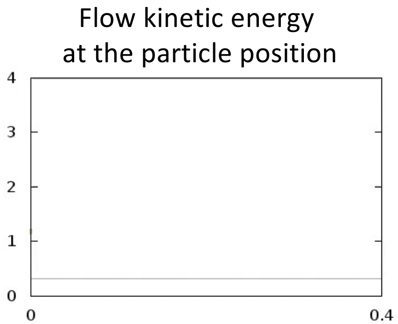




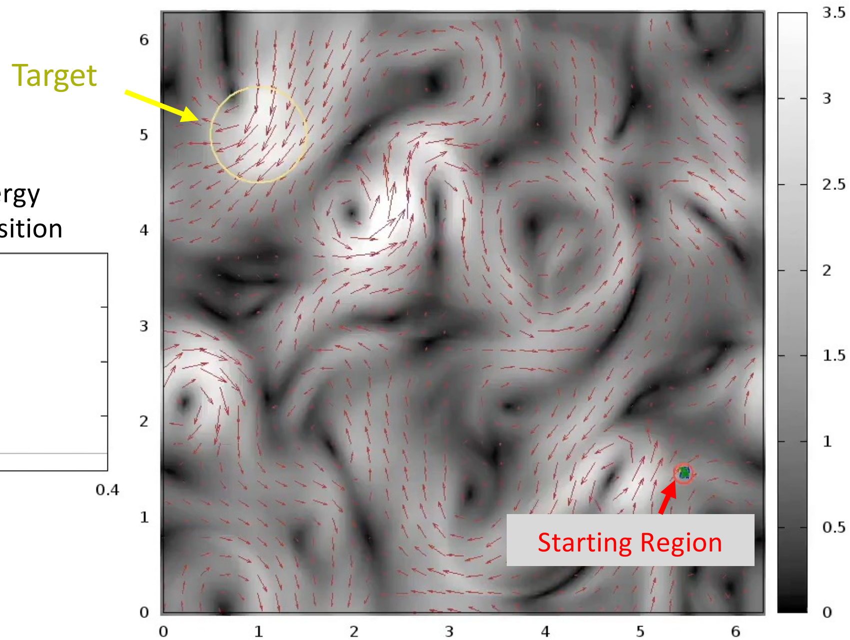
Time-Dependent 2D Turbulent Flow







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



Reinforcement Learning (blue)

vs

Trivial Policy (green)

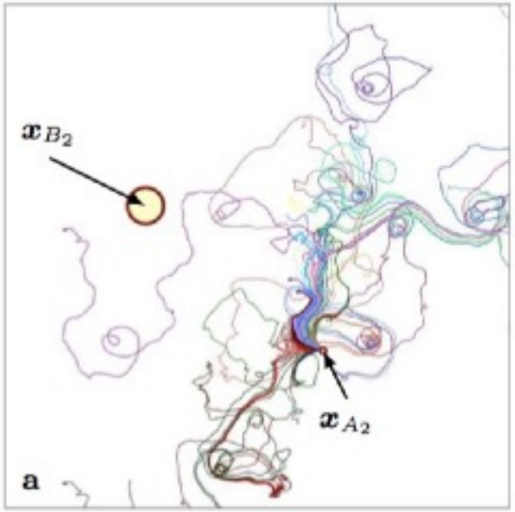
COMPARISON RL VS OPTIMAL NAVIGATION

A. E. Bryson and Y. Ho, Applied optimal control: optimization, estimation and control (New York: Routledge, 1975).

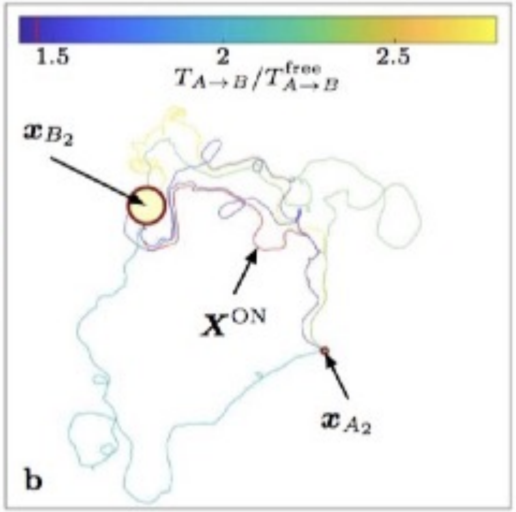
Time independent flow

$$\begin{cases} \dot{\boldsymbol{X}}_t = \boldsymbol{u}(\boldsymbol{X}_t) + \boldsymbol{U}^{ctrl}(\boldsymbol{X}_t) \\ \boldsymbol{U}^{ctrl}(\boldsymbol{X}_t) = V_s \boldsymbol{n}(\boldsymbol{X}_t) \end{cases} \qquad \boldsymbol{n}(\boldsymbol{X}_t) = (\cos[\theta_t], \sin[\theta_t])\,, \quad A_{ij} = \partial_i u_j$$

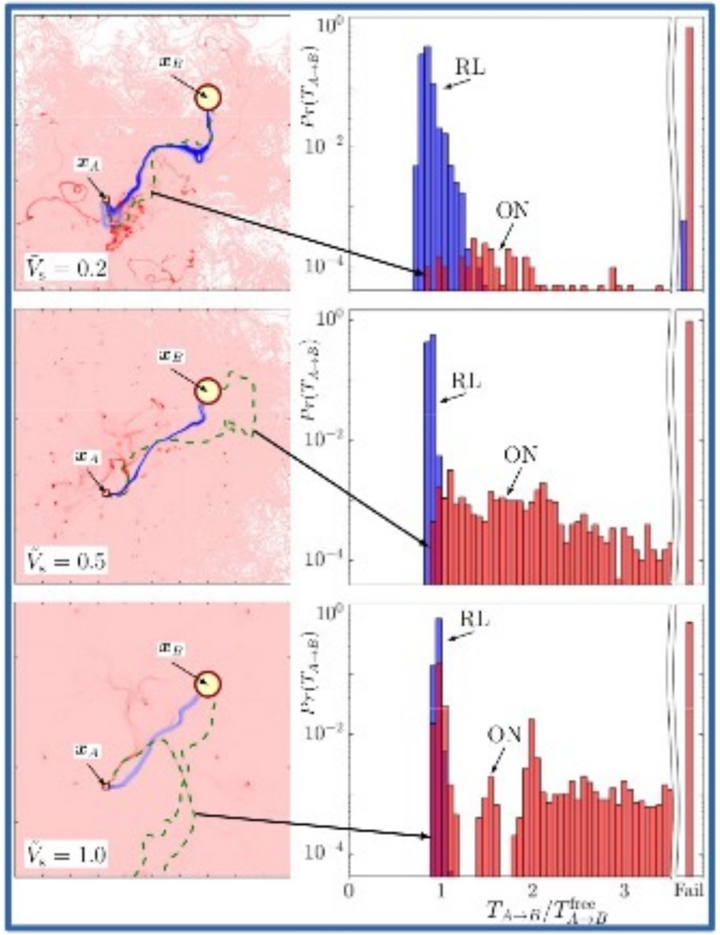
$$\dot{\theta}_t = A_{21} \sin^2 \theta_t - A_{12} \cos^2 \theta_t + (A_{11} - A_{22}) \cos \theta_t \sin \theta_t\,,$$

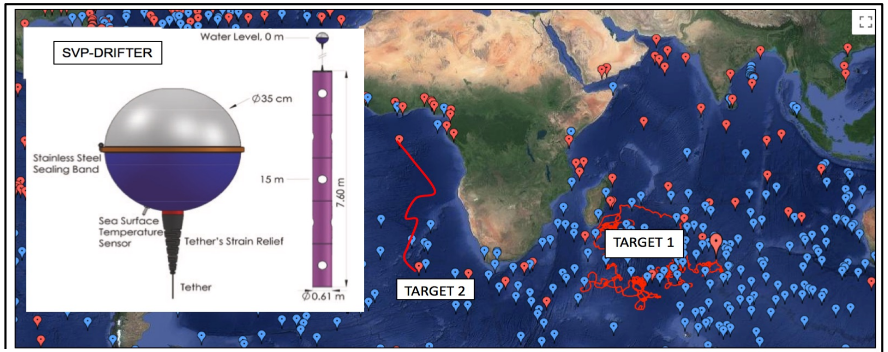


1000 trials (all failures)

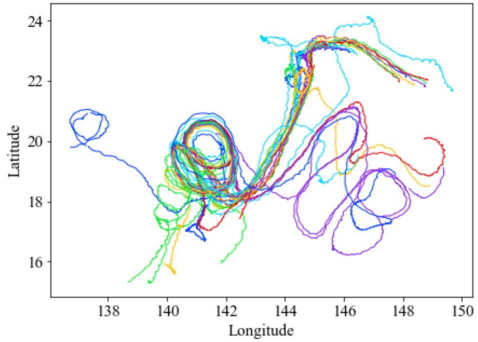


100k trials (10 successes)

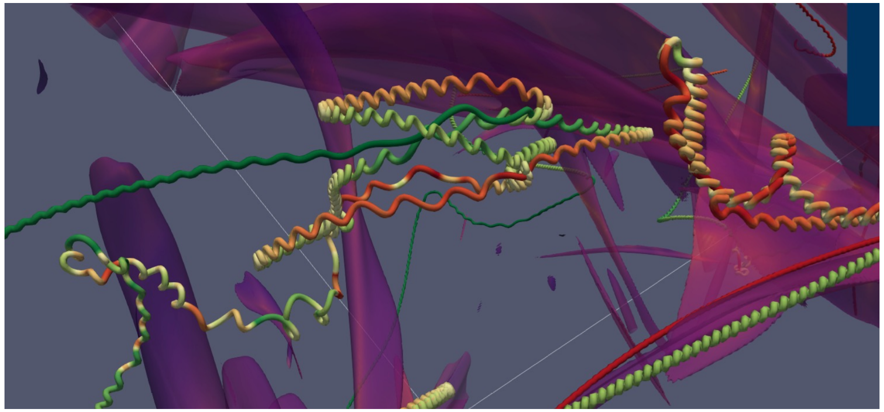




DRIFTERS FROM THE GLOBAL DRIFTER MAP
NTIAL TARGETS: (1) KEEP THE PROBES INSIDE A
AMONG TWO END-POINTS (ZERMELO PROBLEM).
E AT 15M DEPTH.



CHARGED-PARTICLES IN MHD
with RL. Centurioni (UCSD, USA)



CHARGED-PARTICLES IN MHD
with R. Grauer & J. Lubcke (Bochum U., GER)

-WHAT-IF QUESTIONS: EXPLICABILITY OF THE GENERATED DATA, FEATURES RANKINGS, PHYSICS DISCOVERY

Wavelet Score-Based Generative Modeling

Florentin Guth
Computer Science Department,
ENS, CNRS, PSL University

Simon Coste
Computer Science Department,
ENS, CNRS, PSL University

Valentin De Bortoli
Computer Science Department,
ENS, CNRS, PSL University

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WE HAVE NEW TOOLS IN THE BOX!

OPEN ISSUES:

0. EXPLENABILITY. VERY FAR, AT THE MOMENT. COMPUTO ERGO SUM?

1. PROOF-OF-CONCEPTS STAGE. VERY FEW NEW DISCOVERIES/FAR FROM FRONTIER RESEARCH

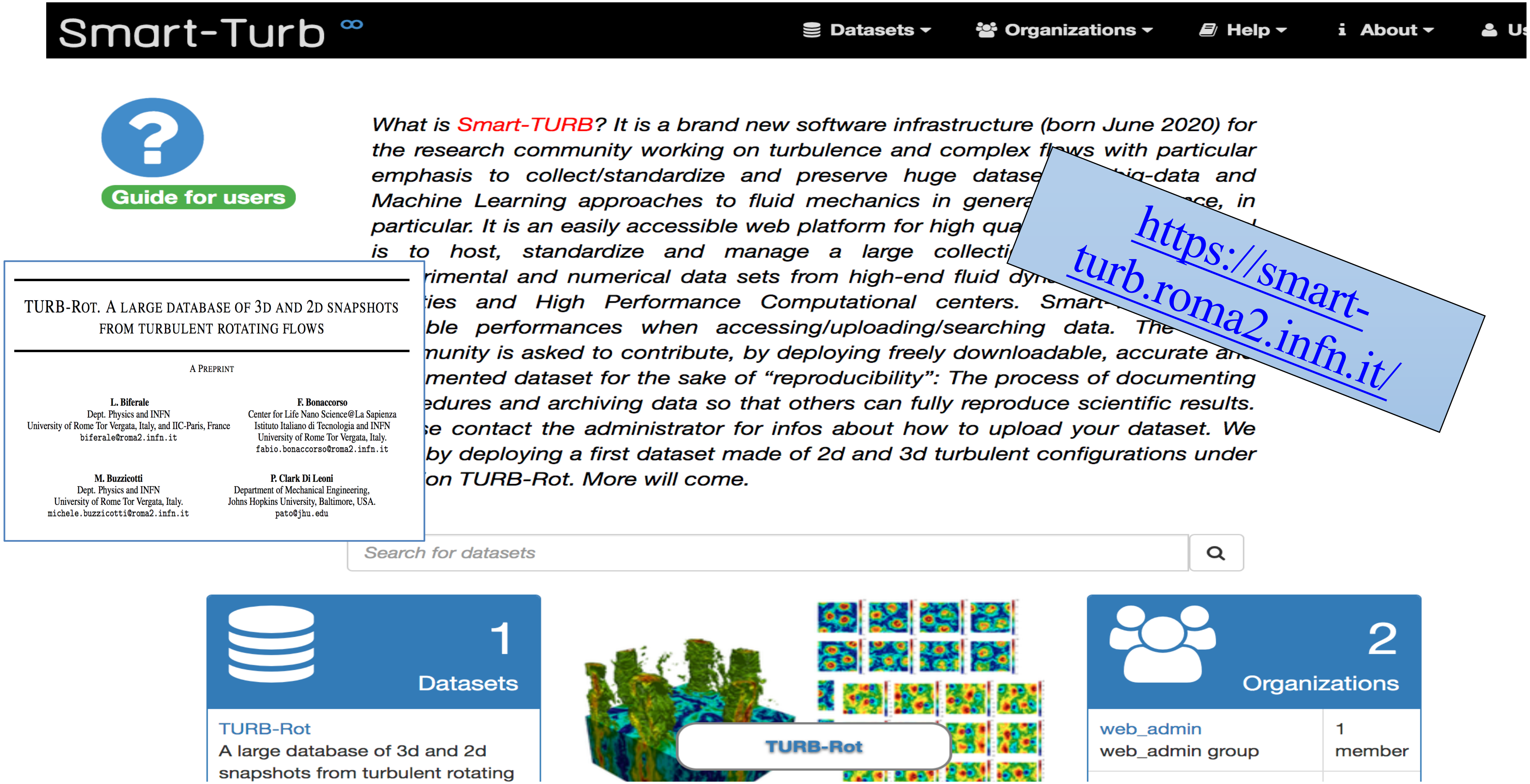
2. GENERALIZABILITY/ROBUSTNESS. CHANGE ANYTHING, CHANGES EVERYTHING?

3. SCALABILITY. VS NETWORK ARCHITECTURE AND VS CONTROL PHYSICAL PARAMETERS

4. UNCERTAINTY QUANTIFICATION/TRUSTABILITY

WHAT WE MISS:

1. COMMUNITY EFFORT TO:
    - (A) DEPLOY AND MAINTAIN HIGH QUALITY AND HIGH QUANTITY DATA (OPEN)
    - (B) IDENTIFY BENCHMARKS, VALIDATION STEPS, BASELINES
    - (C) IDENTIFY GRAND CHALLENGES


Smart-Turb
Datasets
Organizations
Help
About
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 datase
Machine Learning approaches to fluid mechanics in genera
particular. It is an easily accessible web platform for high qua
is to host, standardize and manage a large collecti
rimental and numerical data sets from high-end fluid dyn
ies and High Performance Computational centers. Smart-
ble performances when accessing/uploading/searching data. The
munity is asked to contribute, by deploying freely downloadable, accurate an
mented dataset for the sake of "reproducibility": The process of documenting
edures and archiving data so that others can fully reproduce scientific results.
se contact the administrator for infos about how to upload your dataset. We
by deploying a first dataset made of 2d and 3d turbulent configurations under
on 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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Search for datasets
1
Datasets
TURB-Rot
A large database of 3d and 2d snapshots from turbulent rotating
TURB-Rot
2
Organizations
web_admin
web_admin group
1
member

THANK YOU !

If you are interested to /working in AI applications to fluid dynamics participate to the questionnaire—->

The idea is to survey some information on the subject from the community and present / discuss the results in a JFM Perspective paper

with L. Biferale & M. Buzzicotti

LINK TO THE QUESTIONNAIRE

https://forms.gle/j1ubGQQ8V2S9UwjP8

QR CODE TO REACH THE QUESTIONNAIRE