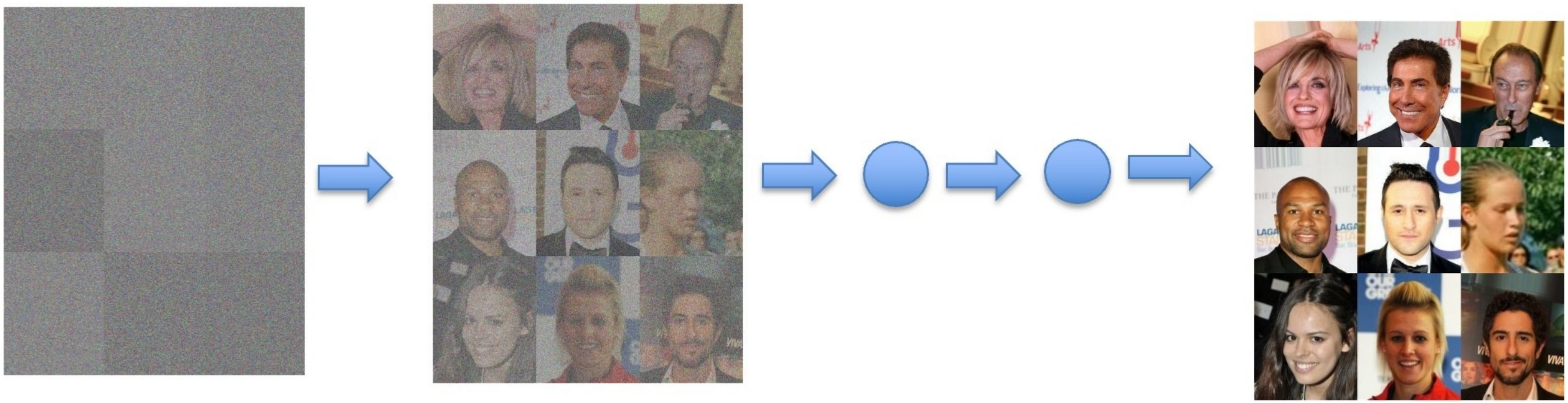
Complex Fluids and Complex Flows Group
Dept. Physics & INFN - University of Rome 'Tor Vergata'
biferale@roma2.infn.it
https://biferale.web.roma2.infn.it/

HOLLYWOOD STARS



ICTS-2023
FIELD THEORY AND TURBULENCE

Data driven tools for Lagrangian Turbulence

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

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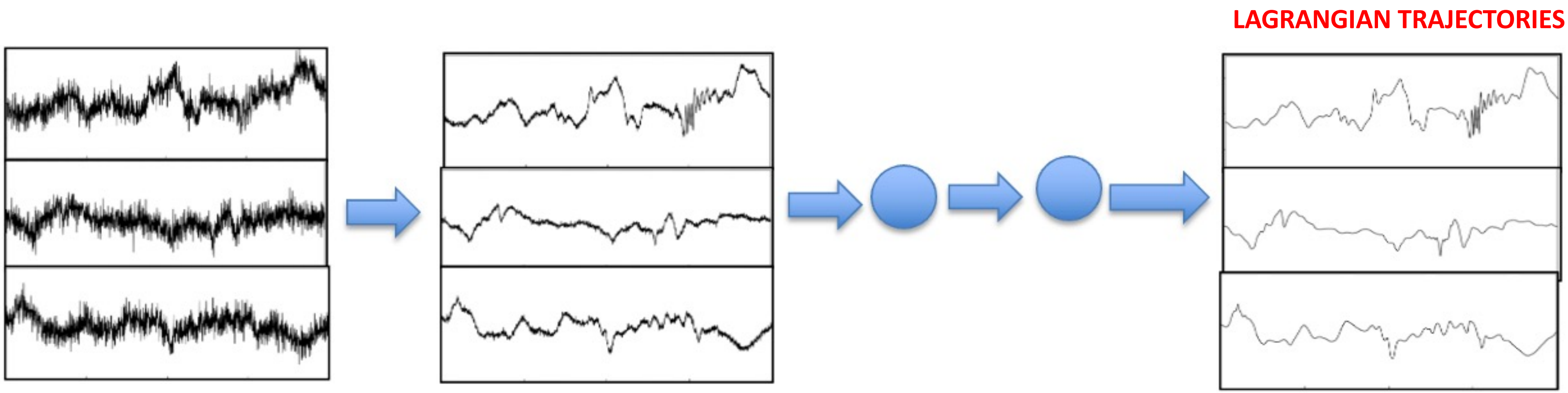


ICTS-2023
FIELD THEORY AND TURBULENCE

Data driven tools for Lagrangian Turbulence

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

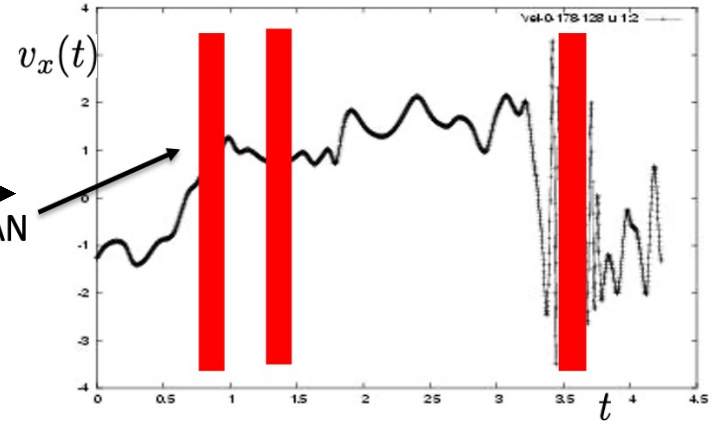
STOCHASTIC MODELS FOR LAGRANGIAN TURBULENCE: WHY?

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

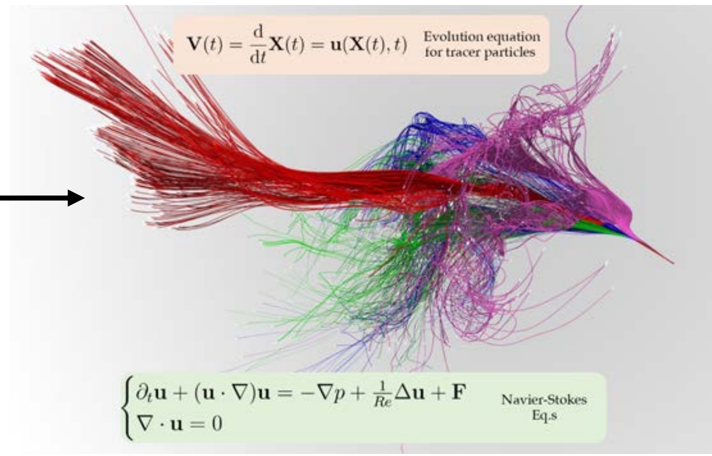
GENERATION OF LARGE SYNTHETIC DATA-BASE FOR
(I) RANKING OF PHYSICS FEATURES
(II) TESTING DOWNSTREAM APPLICATIONS/MODELS

(iii) DATA ASSIMILATION/INPAINTING FROM MISSING FIELD/EXPERIMENTAL OBERVATION

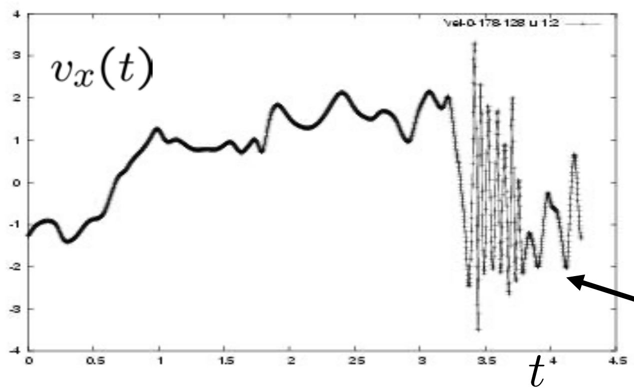
LAGRANGIAN

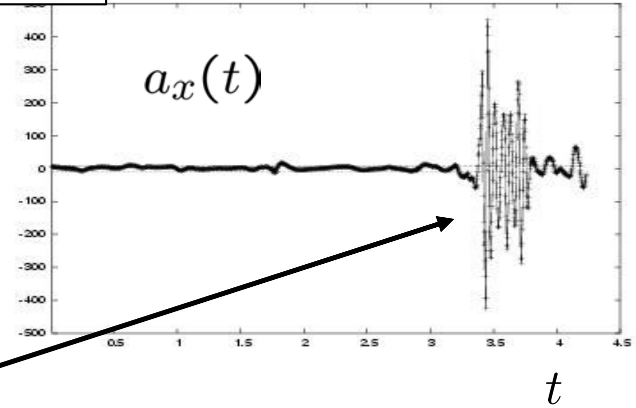


(iv) CLASSIFICATION/INFERRAL OF MISSING/INTERNAL PROPERTIES:
(I) INERTIA
(II) SHAPE
(III) ACTIVE DEGREES OF FREEDOM
(IV) ….

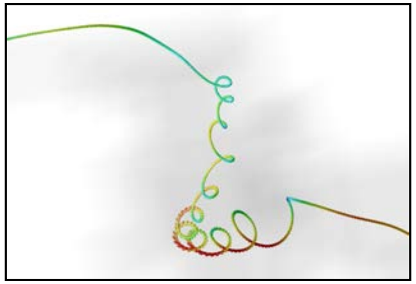


$$\begin{cases} \mathbf{a} = \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \nu\Delta\mathbf{u} + \mathbf{f} \\ \nabla\cdot\mathbf{u} = 0 \end{cases}$$

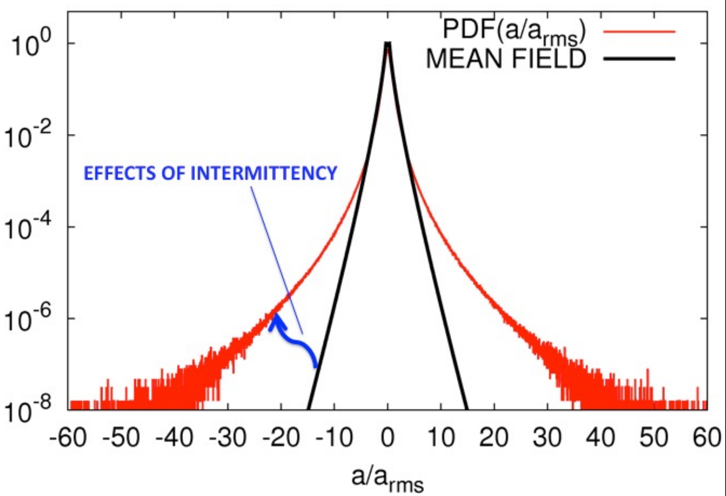




EXTREME EVENTS



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

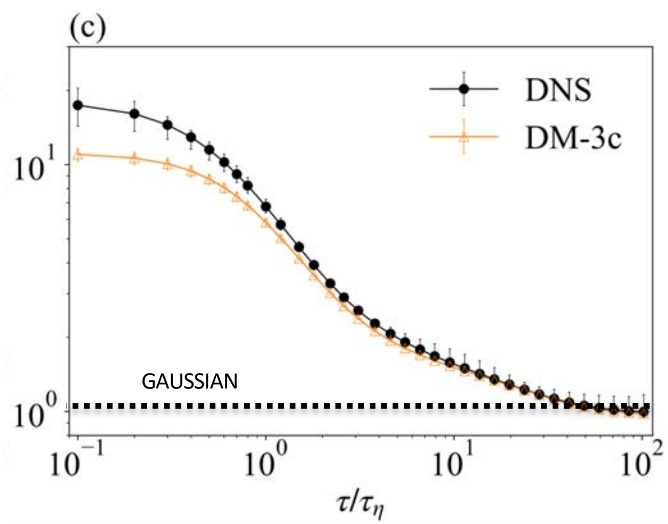


ACCELERATION PROBABILITY DISTRIBUTION FUNCTION (PDF) AT RE ~ 10^5 [Bi04] COMPARED WITH THE PREDICTION FROM MEAN FIELD (KOLMOGOROV THEORY)

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)



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

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

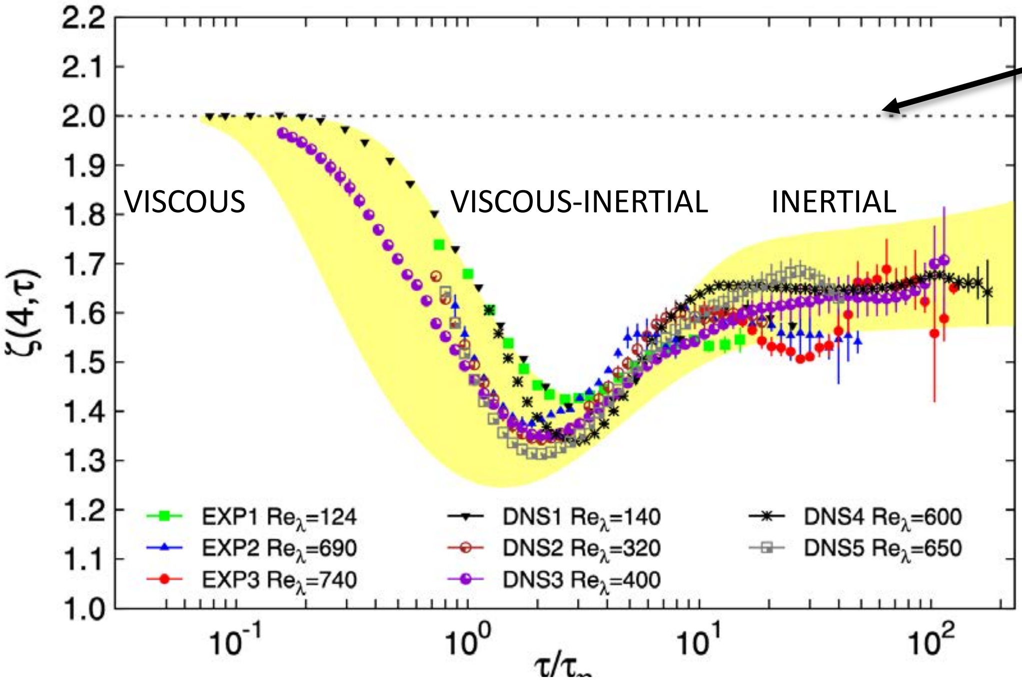
$$\zeta(4,\tau) = \frac{d\log S^{(4)}(\tau)}{d\log S^{(2)}(\tau)}$$

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)

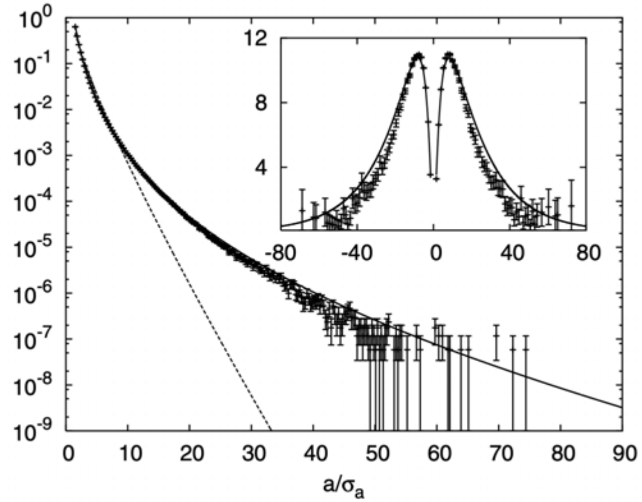


GAUSSIAN – NO INTERMITTENCY

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

$$\delta_\tau v(h) = V_0 \frac{\tau}{T_L}\left[\left(\frac{\tau}{T_L}\right)^\beta + \left(\frac{\tau_\eta}{T_L}\right)^\beta\right]^{(2h-1)/\beta(1-h)}$$

$$\tau_\eta(h)/T_L \sim R_\lambda^{2(h-1)/(1+h)}$$



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)
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Physical Review E 57, R6261 (1998).

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

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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).

Viggiano, B. et al. Modelling lagrangian velocity and acceleration in turbulent flows as infinitely
differentiable stochastic processes. Journal of Fluid Mechanics 900, A27 (2020).

Sinhuber, M., Friedrich, J., Grauer, R. & Wilczek, M. Multi-level stochastic refinement for complex
time series and fields: a data-driven approach. New Journal of Physics 23, 063063 (2021).

Zamansky, R. Acceleration scaling and stochastic dynamics of a fluid particle in turbulence. Physical Review Fluids 7, 084608 (2022).

Lubcke, J, Friedrich, J., Grauer, R. Stochastic interpolation of sparsely sampled time series by a superstatistical random process
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

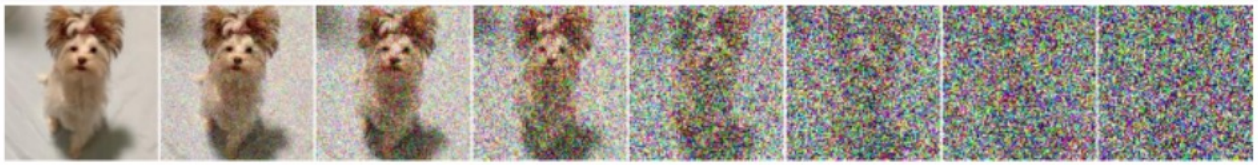
Langevin equation for an Ornstein-Uhlenbeck process

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

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

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

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

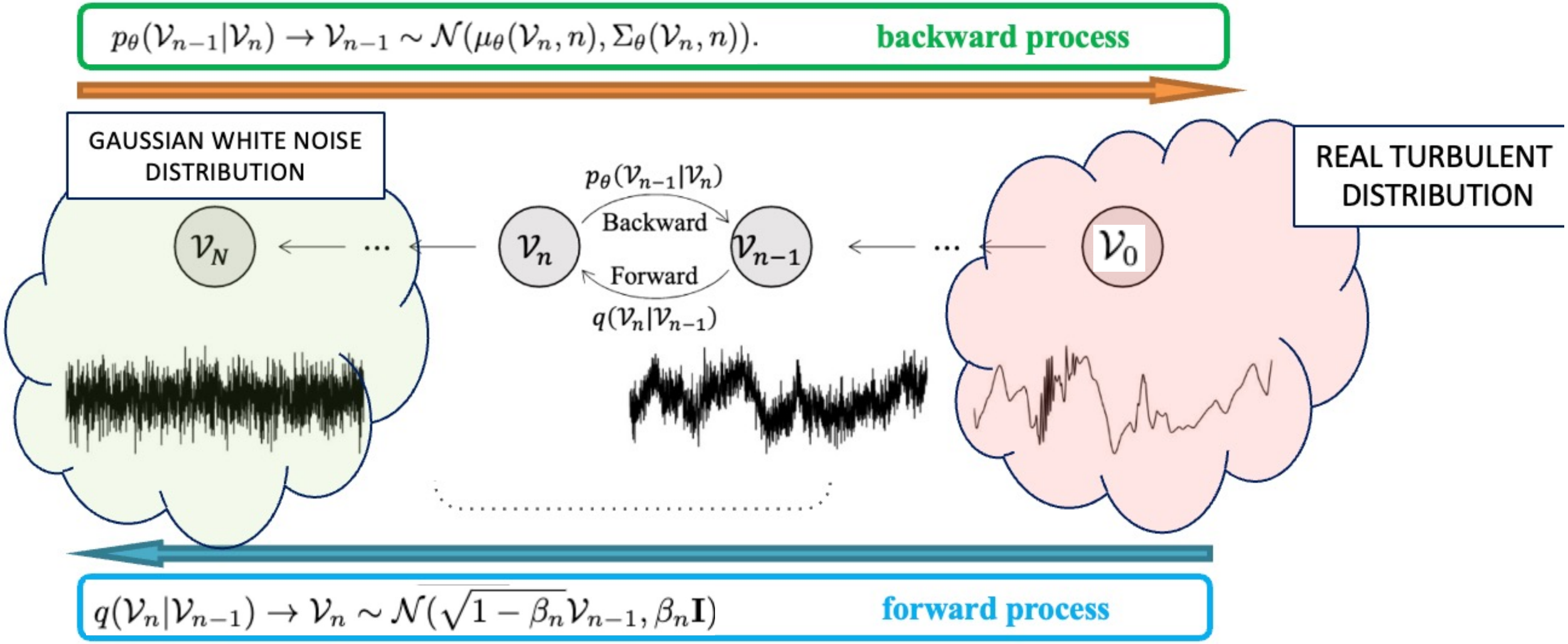


Score function provides the force field to go back in time

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

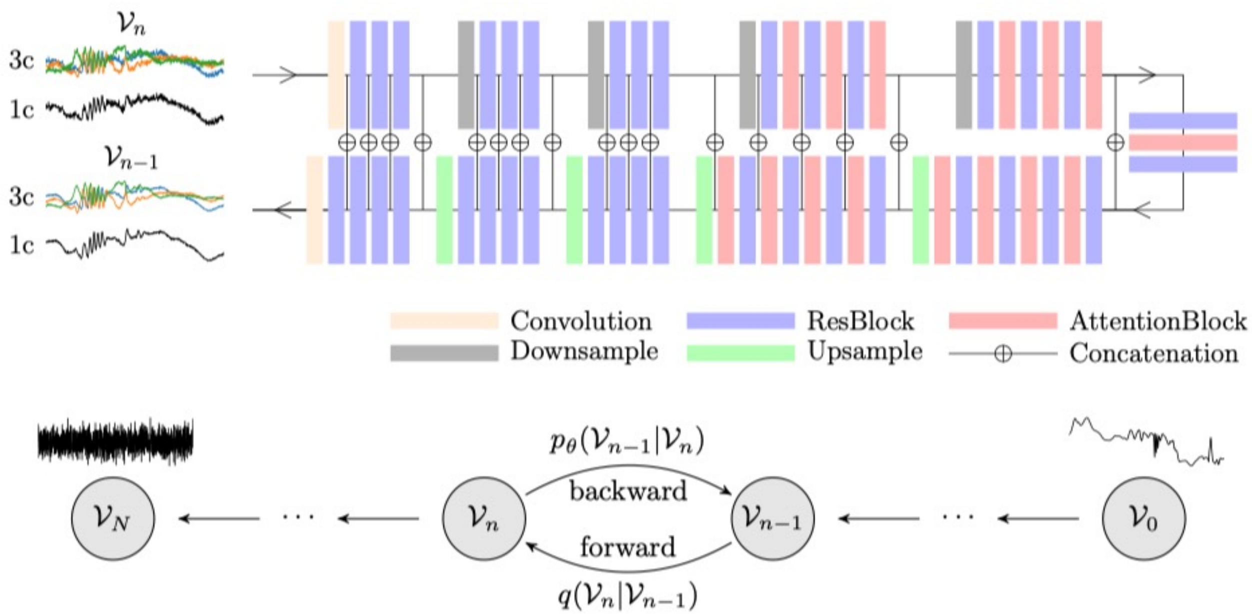
Diffusion Models

'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

(a)

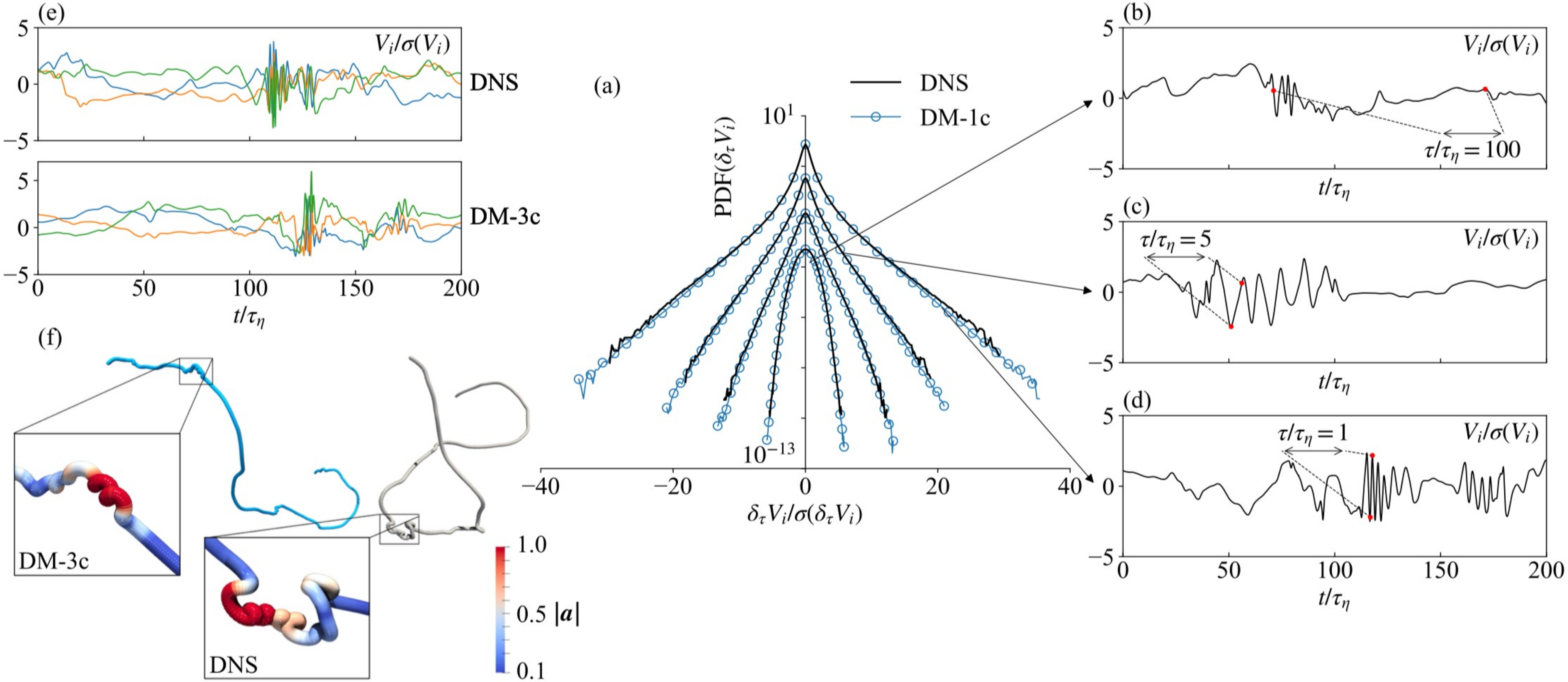


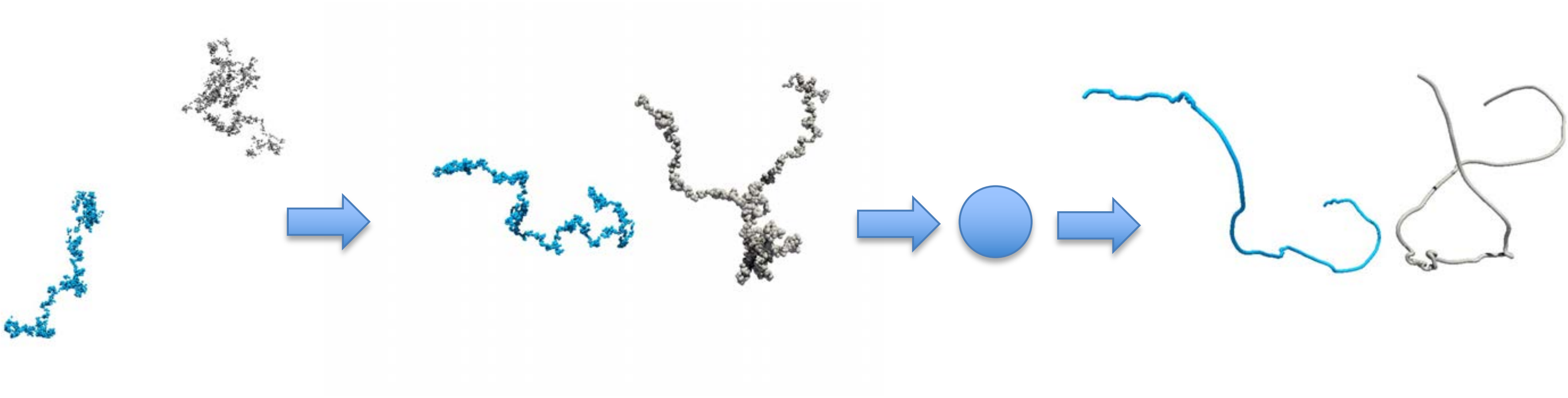
Hyperparameters

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

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

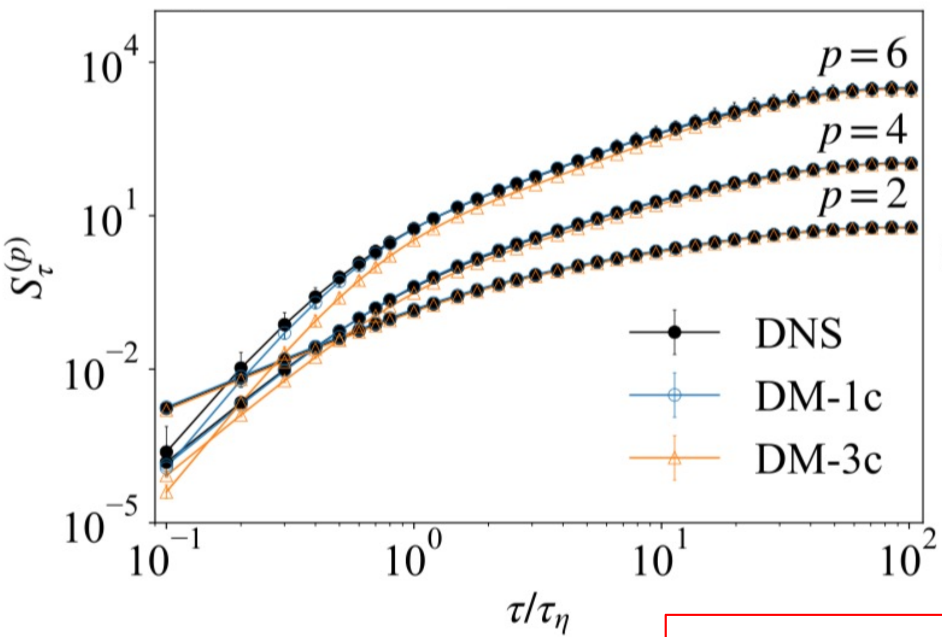
$$\delta_\tau V_i(t) = V_i(t+\tau) - V_i(t),$$





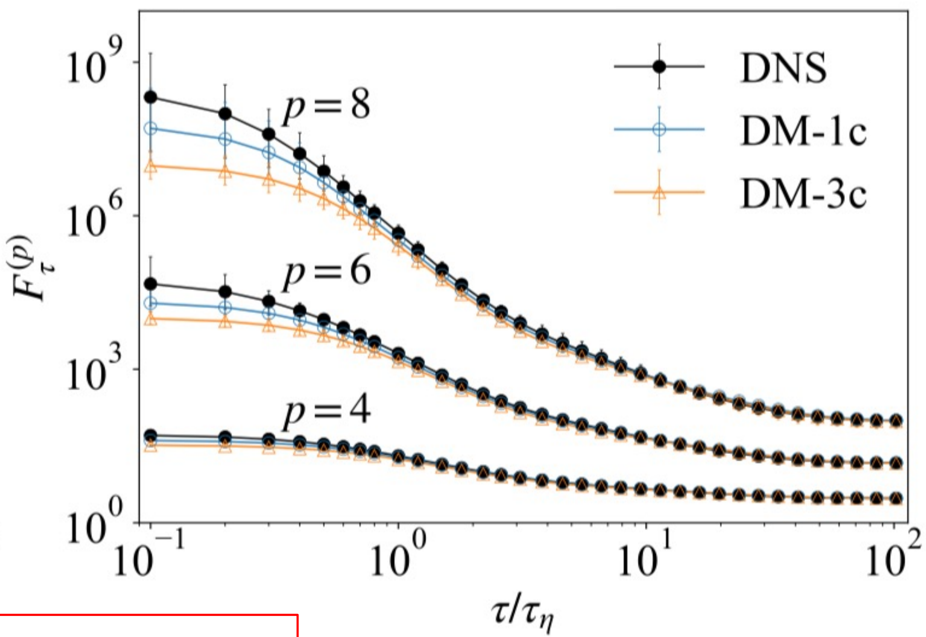
LAGRANGIAN STRUCTURE FUNCTIONS

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

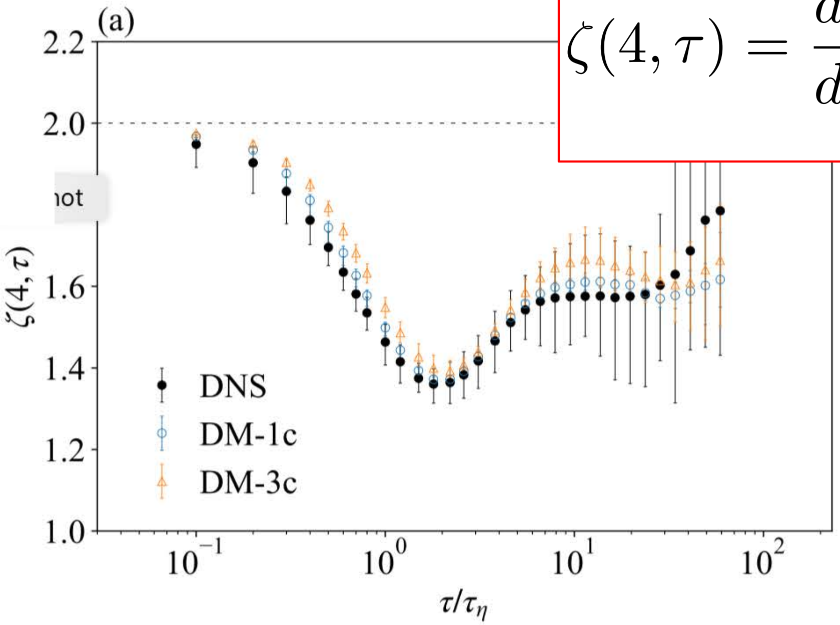


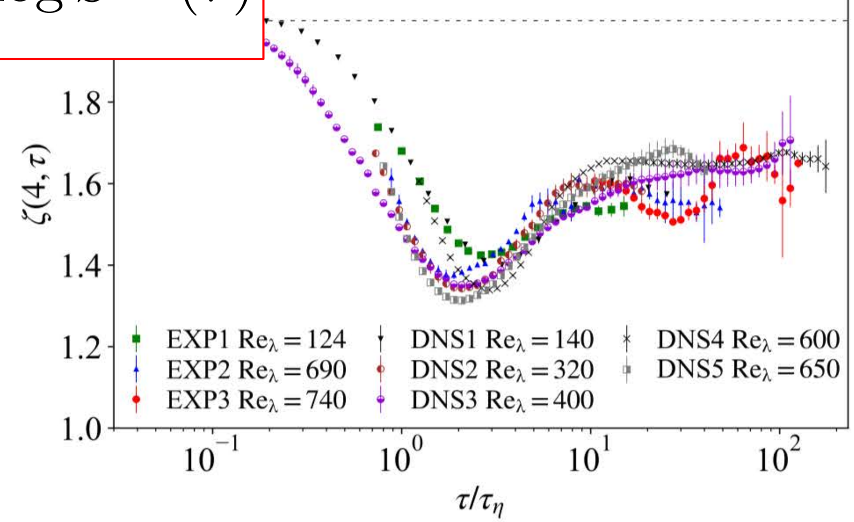
GENERALIZED FLATNESS

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

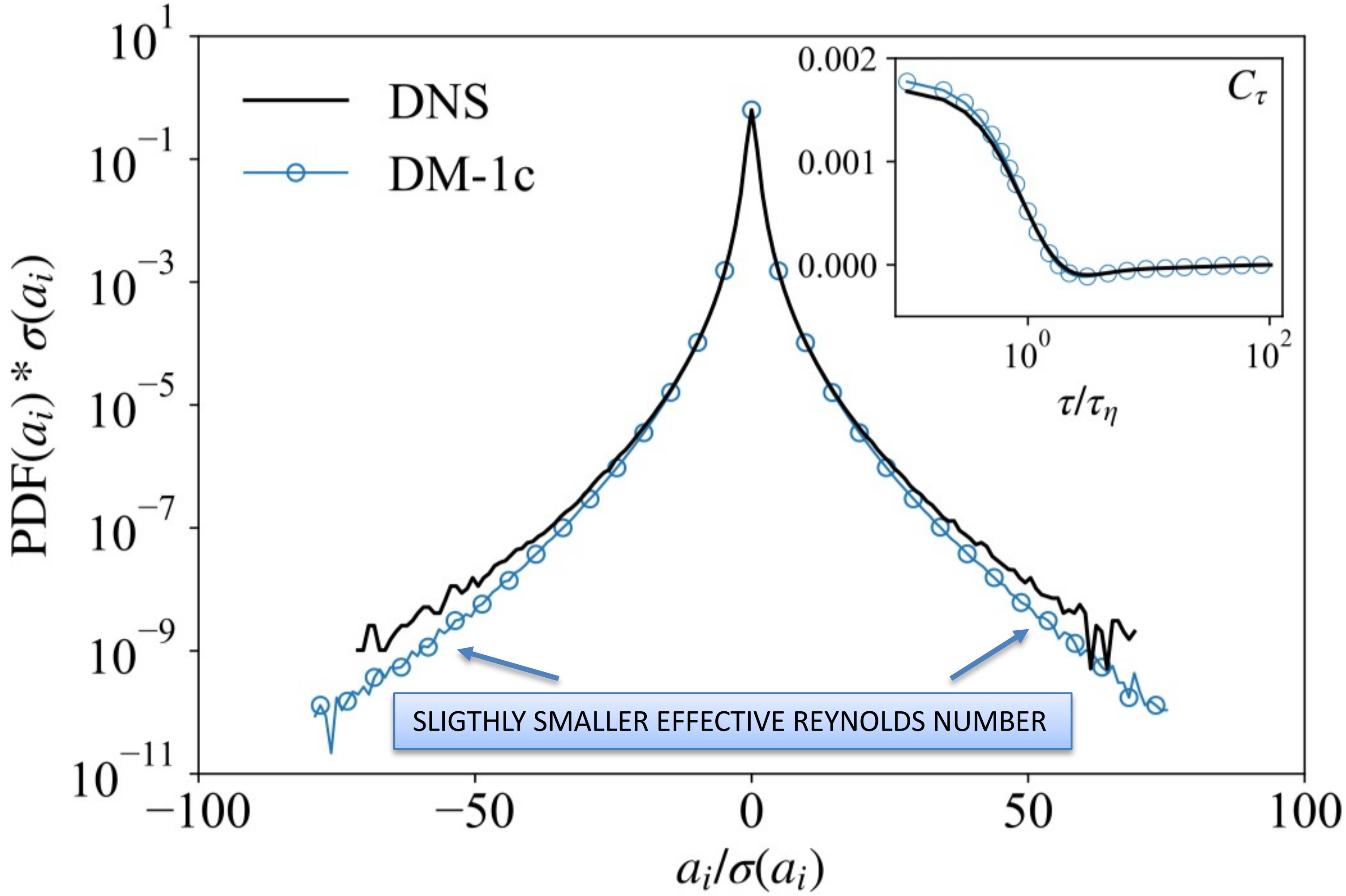


$$\boxed{\zeta(4,\tau) = \frac{d \log S^{(4)}(\tau)}{d \log S^{(2)}(\tau)}}$$

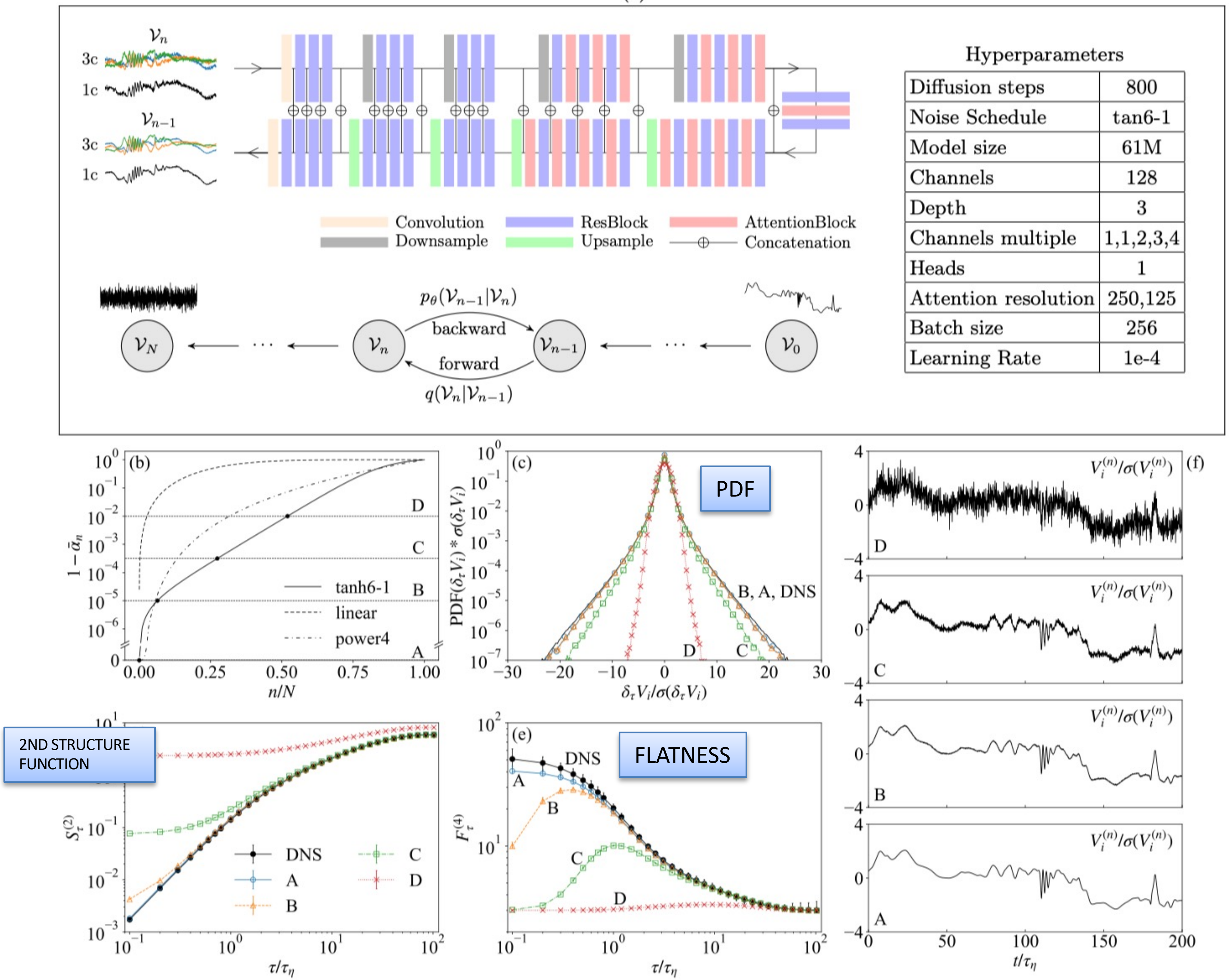




ACCELERATION PDF



(a)



Hyperparameters	
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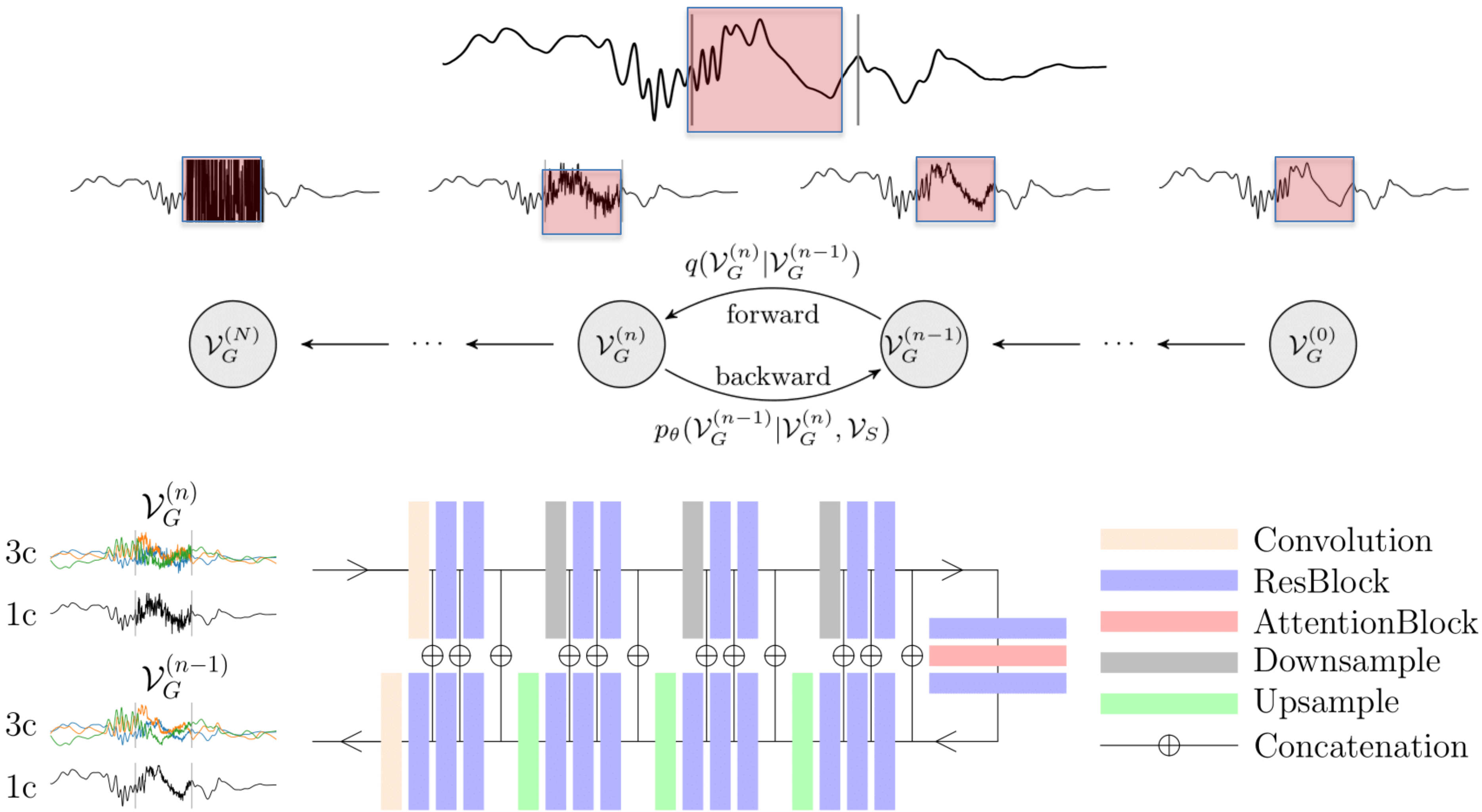
Depth	3
Channels multiple	1,1,2,3,4
Heads	1
Attention resolution	250,125
Batch size	256
Learning Rate	1e-4

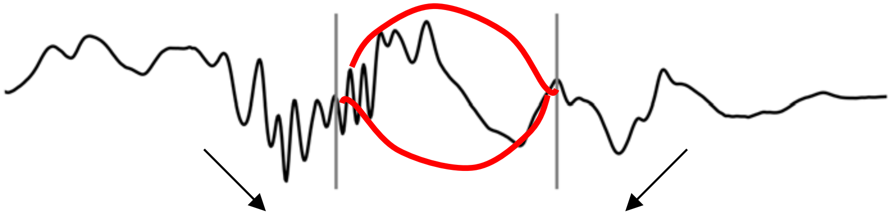
IMPUTATION OF LAGRANGIAN TRAJECTORIES: CONDITIONAL DM

Gap size: $T_G/\tau_\eta = 50, T_G/T_I = 1/4$



Gaussian Process Regression (GPR)

Gap region, G



Measurement region, S

Training process:

$$\mathcal{V}_S = \{V(t_{s_1}), V(t_{s_2}), \dots, V(t_{s_{N(S)}}) \,|\, t_{s_i} \in S\}$$

$$\mathcal{V}_G = \{V(t_{g_1}), V(t_{g_2}), \dots, V(t_{g_{N(G)}}) \,|\, t_{g_i} \in G\}$$

$$\begin{bmatrix} \mathcal{V}_S \\ \mathcal{V}_G \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} C_{SS} & C_{SG} \\ C_{GS} & C_{GG} \end{bmatrix}\right)$$

$$(C_{SS})_{ij} = \langle V(t_{s_i}) V(t_{s_j}) \rangle$$

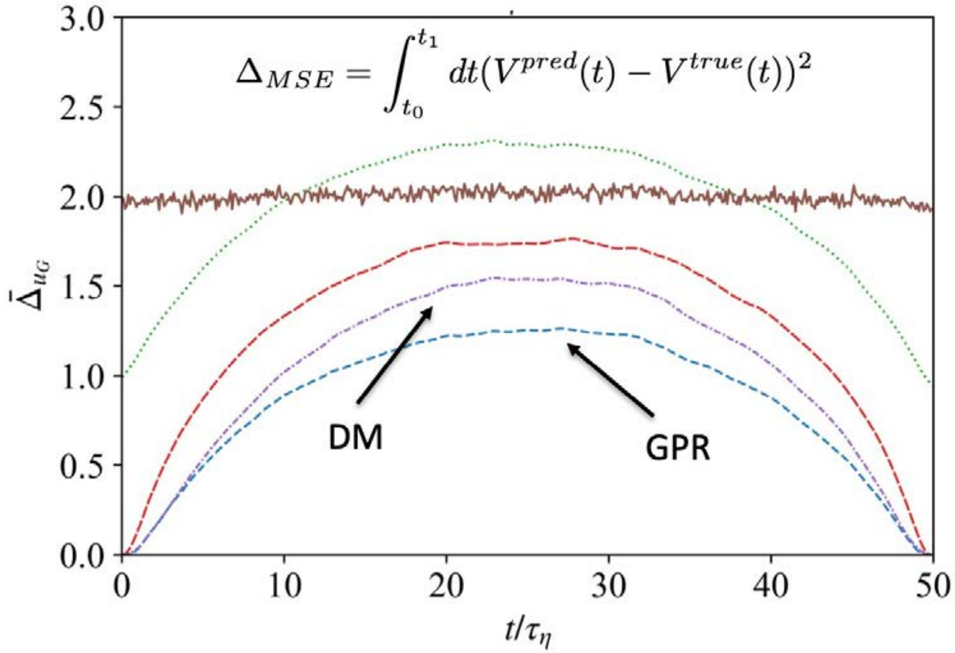
computing the covariance with training data

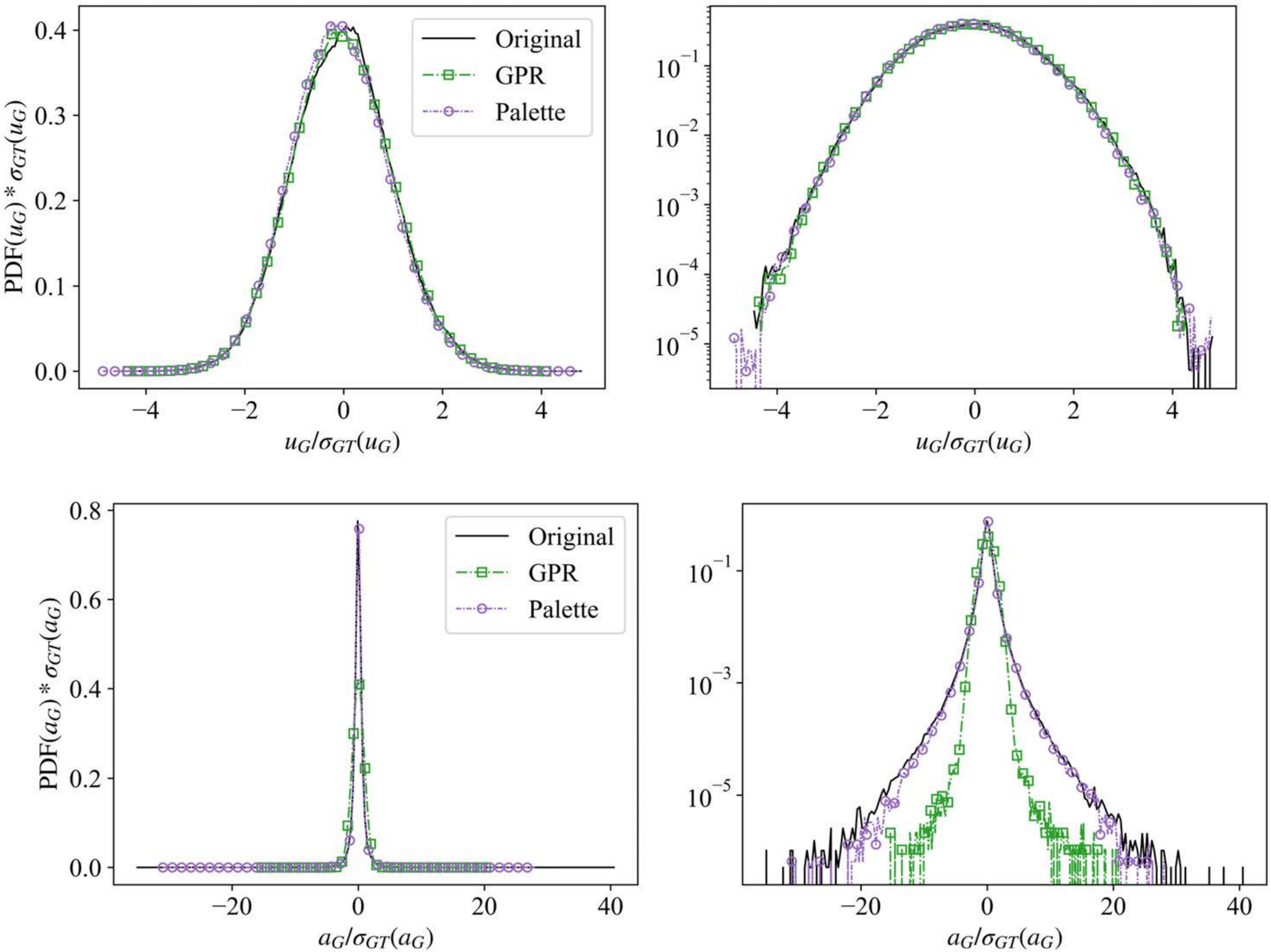
Reconstruction with measurement, $\mathcal{V}_S$:

$$\mathcal{V}_G | \mathcal{V}_S \sim \mathcal{N}(\mu_G, \Sigma_{GG})$$

$$\mu_G = C_{GS} C_{SS}^{-1} \mathcal{V}_S$$

$$\Sigma_{GG} = C_{GG} - C_{GS} C_{SS}^{-1} C_{SG}$$



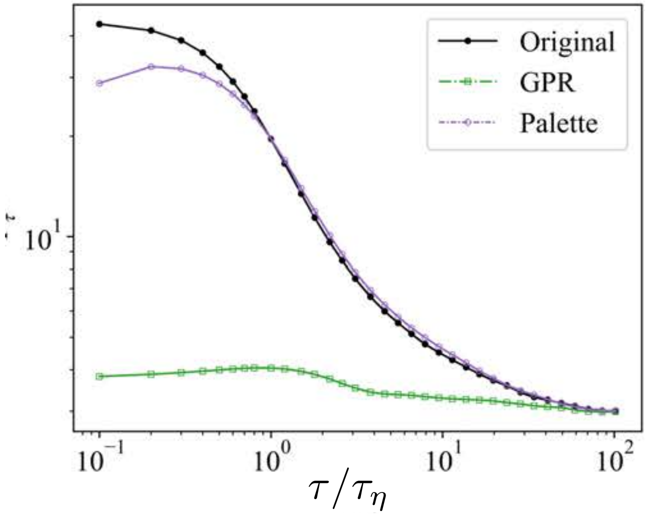


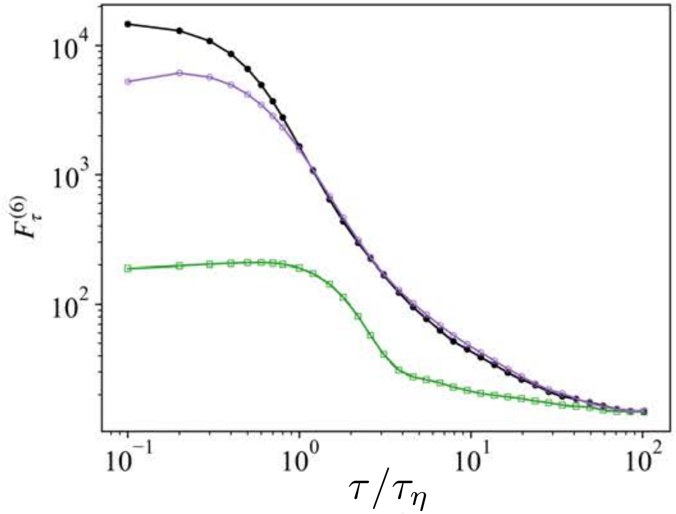
Original
GPR
Palette
PDF(u_G) * $\sigma_{GT}(u_G)$
$u_G/\sigma_{GT}(u_G)$
PDF(a_G) * $\sigma_{GT}(a_G)$
$a_G/\sigma_{GT}(a_G)$

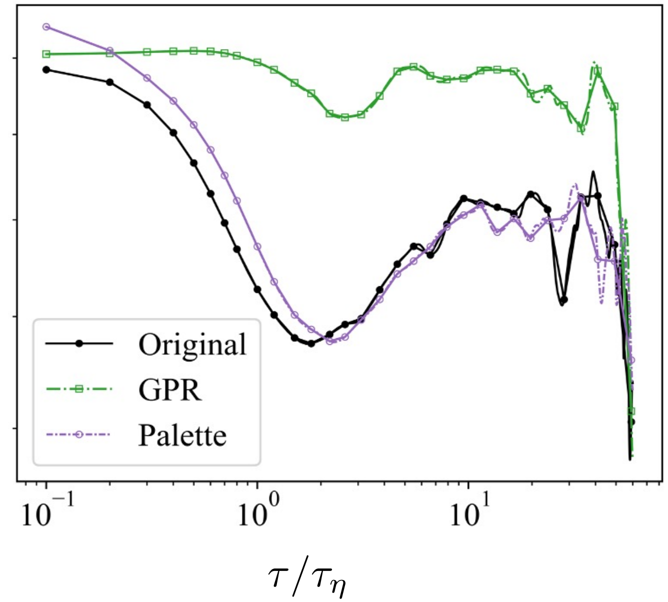
$$F(\tau) = \frac{S^{(4)}(\tau)}{[S^{(2)}(\tau)]^2}$$

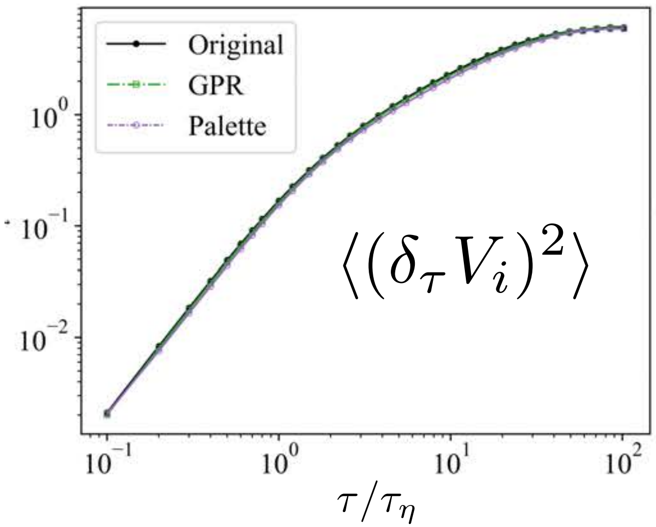
$$F(\tau) = \frac{S^{(6)}}{[S^{(2)}]^3}$$

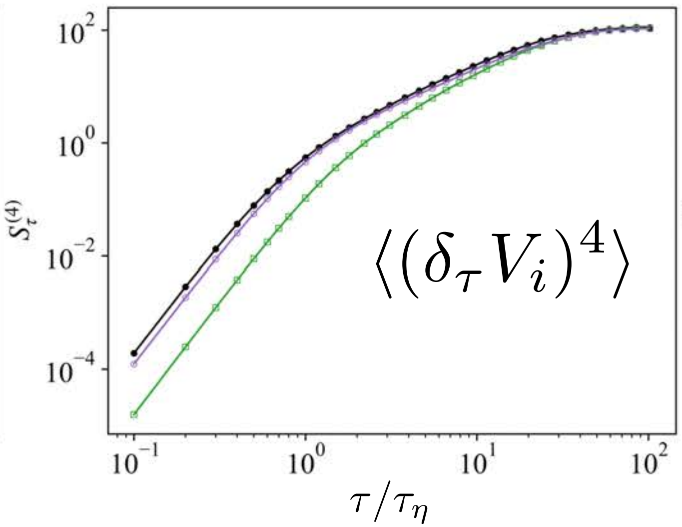
$$\zeta(p,\tau) = \frac{d\ \log S_\tau^{(p)}}{d\ \log S_\tau^{(2)}}.$$



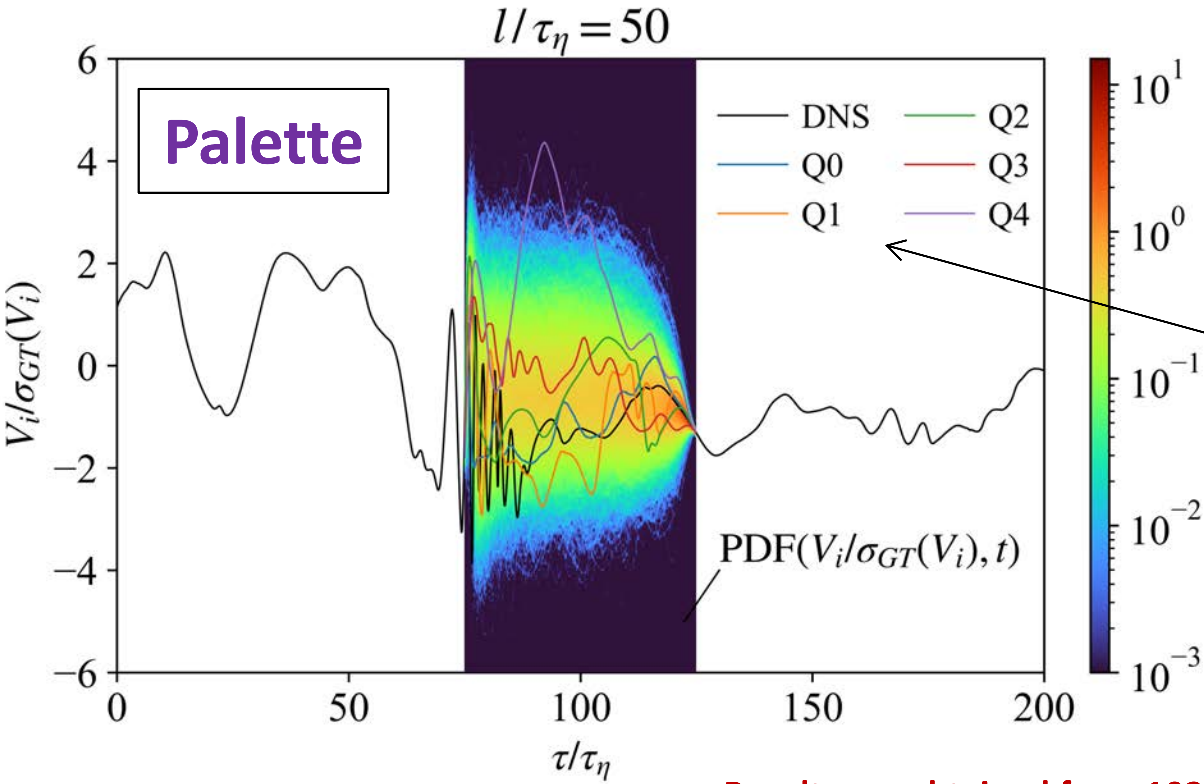


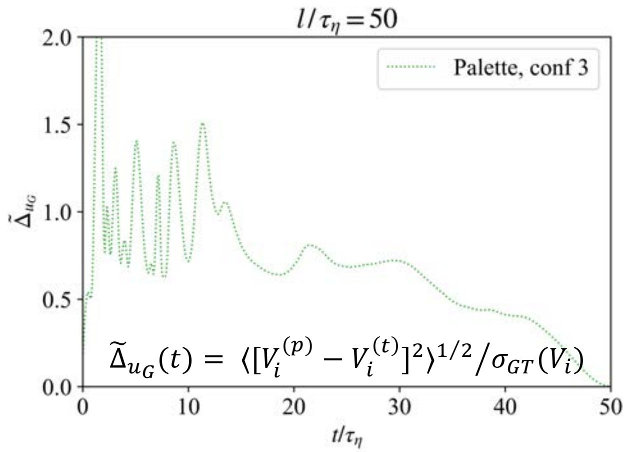


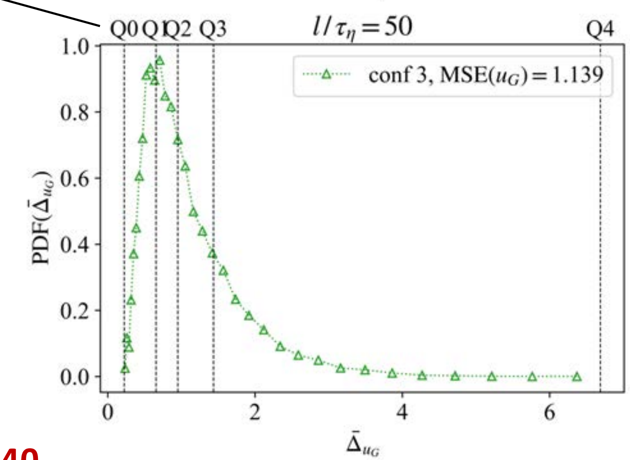




Probabilistic reconstruction

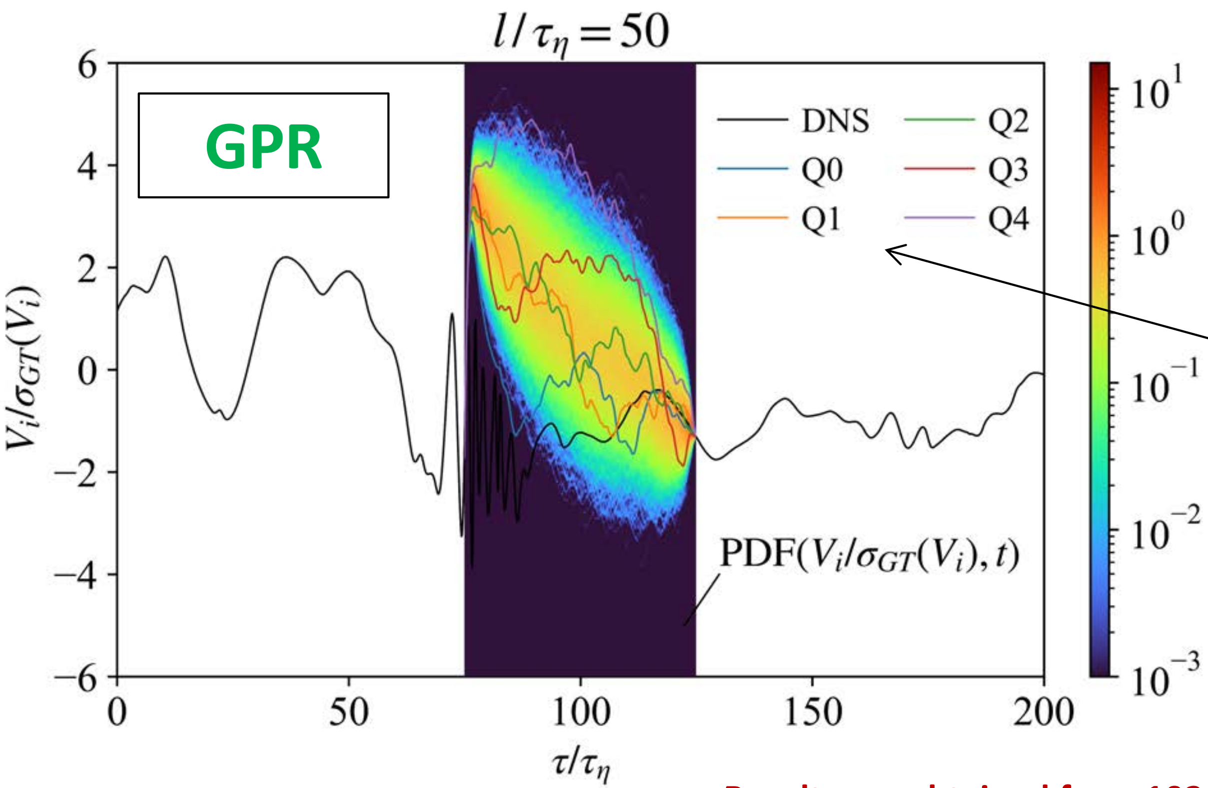


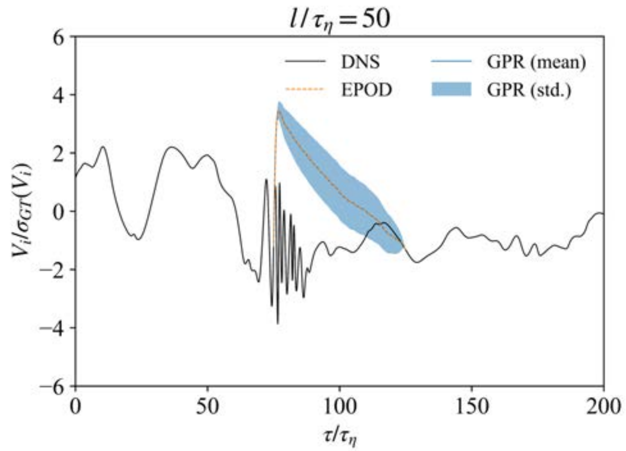


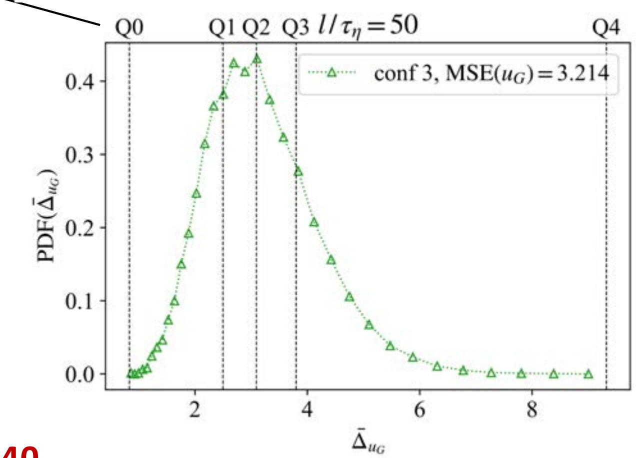


Results are obtained from 10240
independent reconstructions
for the same measurement

Probabilistic reconstruction

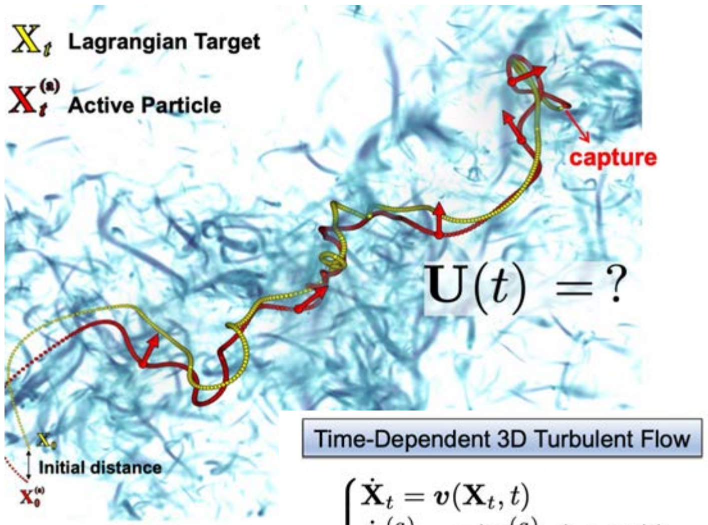






Results are obtained from 10240
independent reconstructions
for the same measurement

OPTIMAL NAVIGATION POLICIES OF LAGRANGIAN ACTIVE SMALL OBJECTS

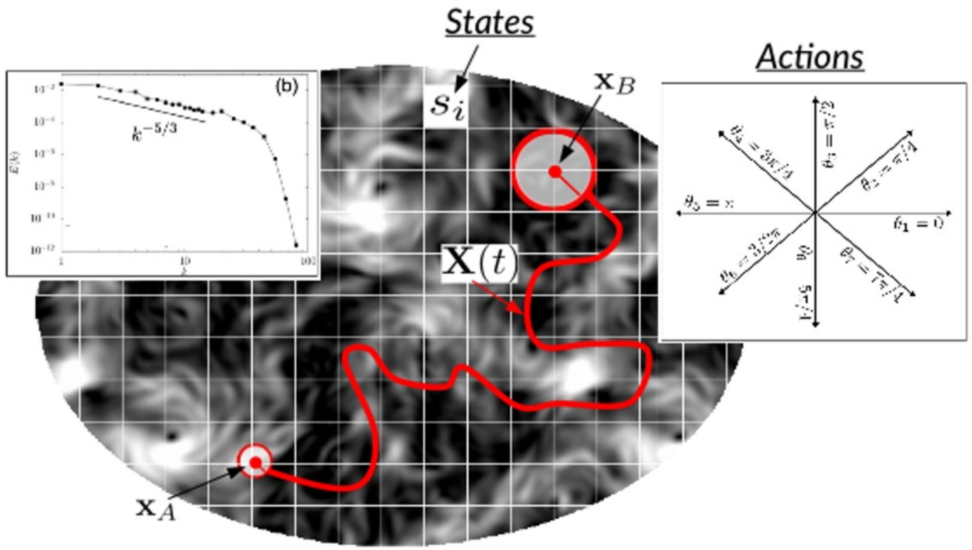


$$\begin{cases} \dot{\mathbf{X}}_t = \boldsymbol{v}(\mathbf{X}_t, t) \\ \dot{\mathbf{X}}_t^{(a)} = \boldsymbol{v}(\mathbf{X}_t^{(a)}, t) + \mathbf{U}(t) \\ \mathbf{U}(t) = V_s \hat{\boldsymbol{n}}(t) \end{cases}$$

Small active control compared to the underling flow!

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

Reinforcement Learning; *Policy Gradient Methods*



Optimal tracking strategies in a turbulent flow. Calascibetta, C., B. L., Borra, F. *et al.* *Commun Phys* **6**, 256 (2023).

Zermelo's problem: optimal point-to-point navigation in 2D turbulent flows using reinforcement learning. L B. F Bonaccorso, M Buzzicotti, P Clark Di Leoni, K Gustavsson Chaos: An Interdisciplinary Journal of Nonlinear Science 29 (2019)

(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 $\dot{\mathbf{X}}_t = \boldsymbol{f}(\mathbf{X}(t), \mathbf{U}(t), t)$

and other possible constraints,

e.g.: $\begin{cases} \mathbf{X}(t_f) = \mathbf{X}_\star\,, \quad \mathbf{X}(t_0) \le \mathbf{X}_\star\,, \\ \|\mathbf{U}(t)\|^2 = 1\,, \quad \|\mathbf{U}(t)\|^2 \le 1\,, \text{ exc.} \end{cases}$

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

$\|\boldsymbol{R}_{t_0}\| \sim \dfrac{V_s}{\lambda_{lyapunov}}$ border of controllability

In our case:

capture's distance

$\|\boldsymbol{R}^\star\| = \|\boldsymbol{R}_{t_0}\|/100$

Minimiz
e $J = \|\boldsymbol{R}_{t_f}\|^2 + c\int_{t_0}^{t_f} dt\, \theta(\|\boldsymbol{R}_{t_f}\|^2 - \|\boldsymbol{R}^\star\|^2)$

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

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

Minimize trajectories' separation

Minimize time of arrival at the desired distance

(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 $\dot{\mathbf{X}}_t = \boldsymbol{f}(\mathbf{X}(t), \mathbf{U}(t), t)$

and other possible constraints,

e.g.: $\begin{cases} \mathbf{X}(t_f) = \mathbf{X}_\star\,, \quad \mathbf{X}(t_0) \le \mathbf{X}_\star\,, \\ \|\mathbf{U}(t)\|^2 = 1\,, \quad \|\mathbf{U}(t)\|^2 \le 1\,, \text{ exc.} \end{cases}$

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

$\|\boldsymbol{R}_{t_0}\| \sim \dfrac{V_s}{\lambda_{lyapunov}}$ border of controllability

In our case:

capture's distance

$\|\boldsymbol{R}^\star\| = \|\boldsymbol{R}_{t_0}\|/100$

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

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

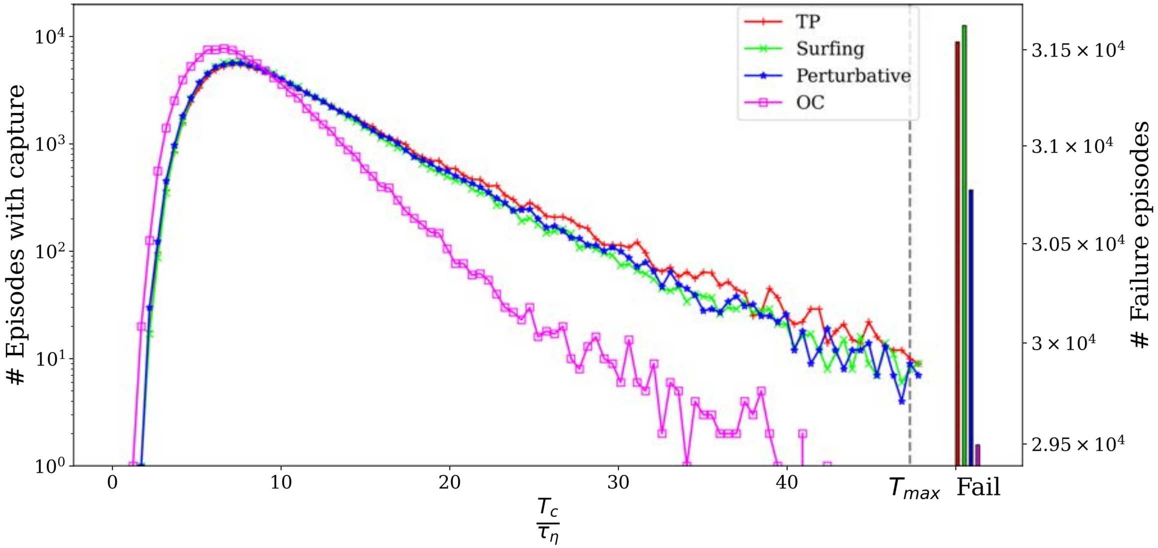
$$\begin{cases} \dot{\boldsymbol{R}}_t = \nabla \boldsymbol{v}_t \boldsymbol{R}_t + \mathbf{U}(t)\,, \\ \mathbf{U}(t) = V_S \hat{\boldsymbol{n}}(t)\,. \end{cases} \qquad (2)$$

LINEAR REGIME

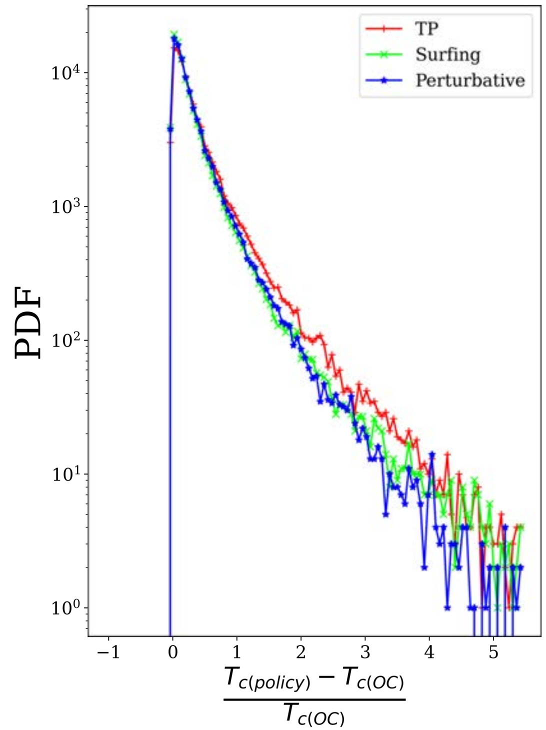
Optimal Control vs heuristic policies in linear regime

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

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



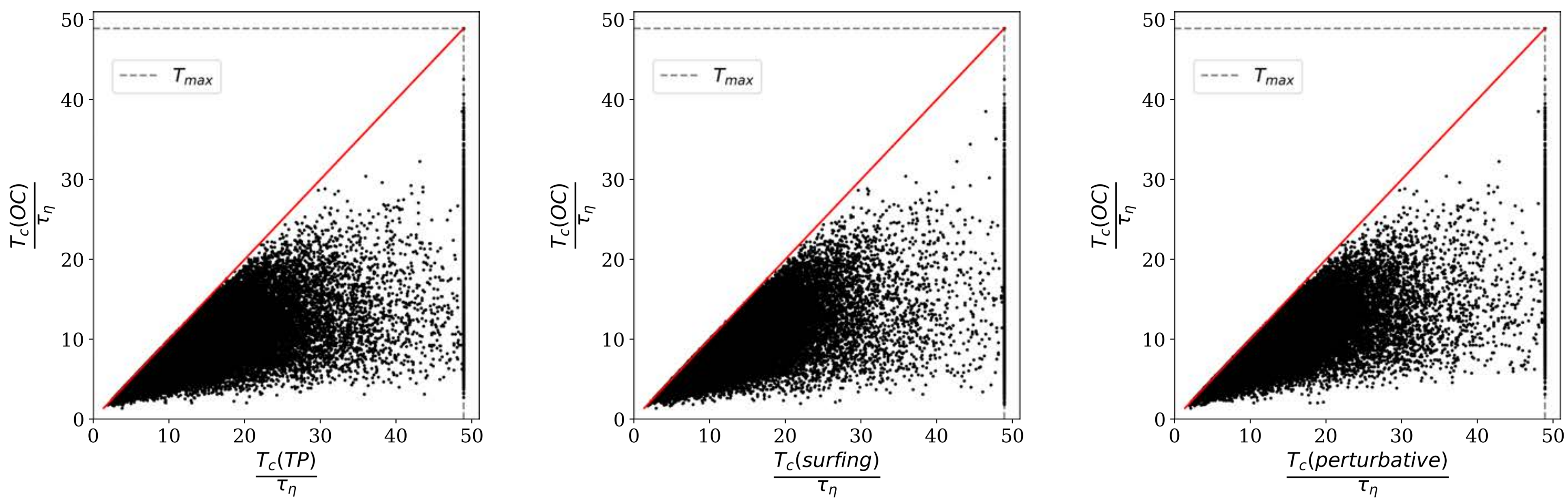
PDF of normalized capture time

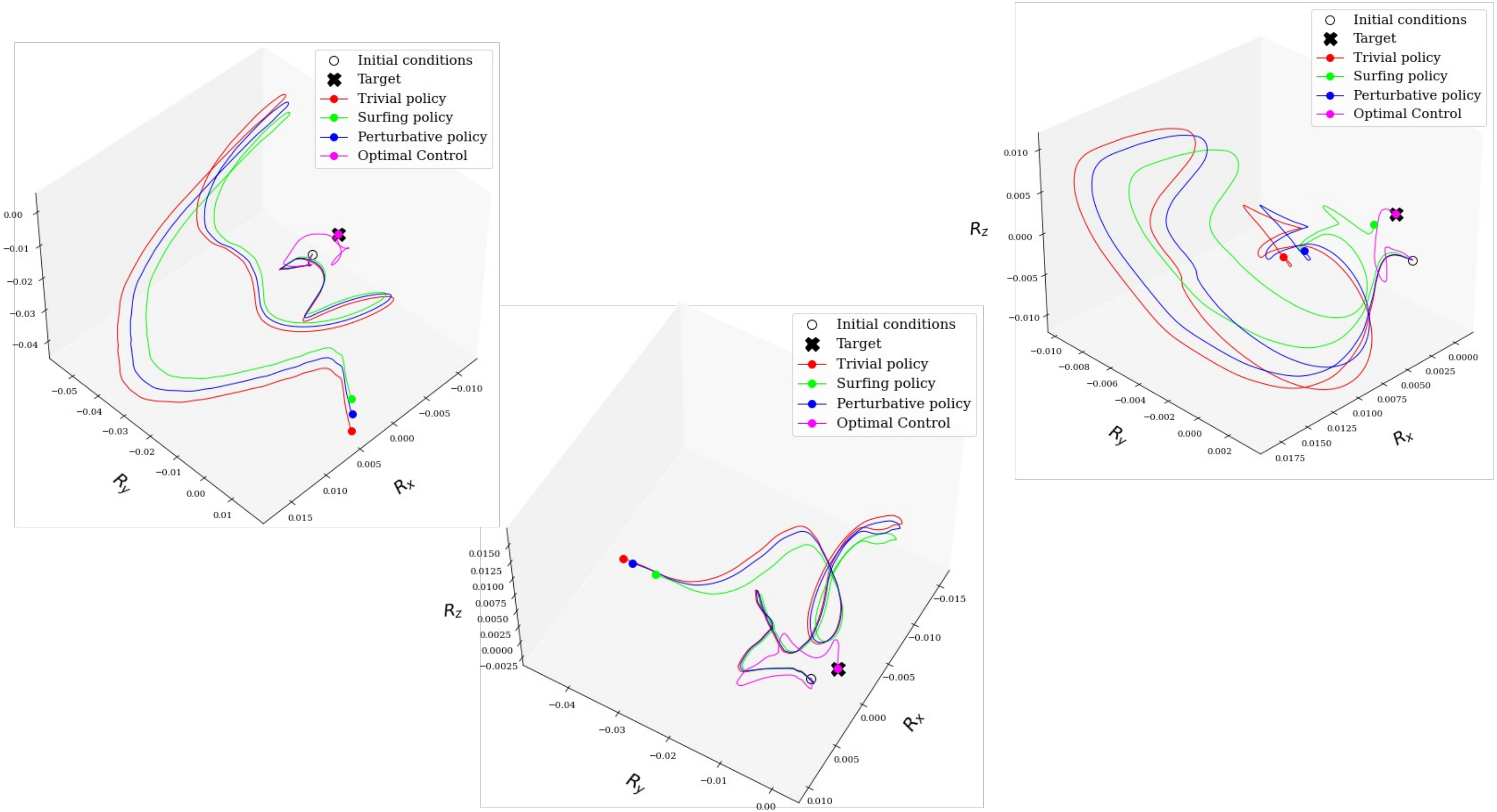


Optimal Control vs heuristic policies at **small scales**

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

$T_c =$ **Capture** time: (time of arriving at the desired distance)

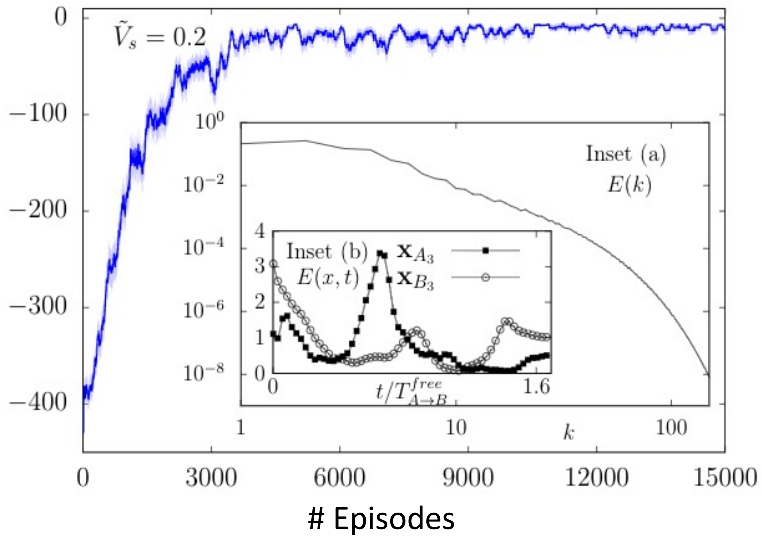


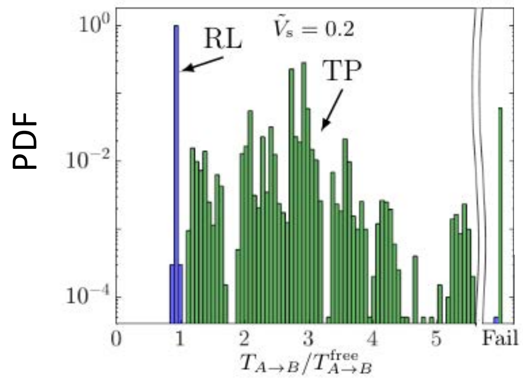


Initial conditions
Target
Trivial policy
Surfing policy
Perturbative policy
Optimal Control
R_z
R_y
R_x
Initial conditions
Target
Trivial policy
Surfing policy
Perturbative policy
Optimal Control
R_z
R_y
R_x
Initial conditions
Target
Trivial policy
Surfing policy
Perturbative policy
Optimal Control
R_z
R_y
R_x

Time-Dependent 2D Turbulent Flow

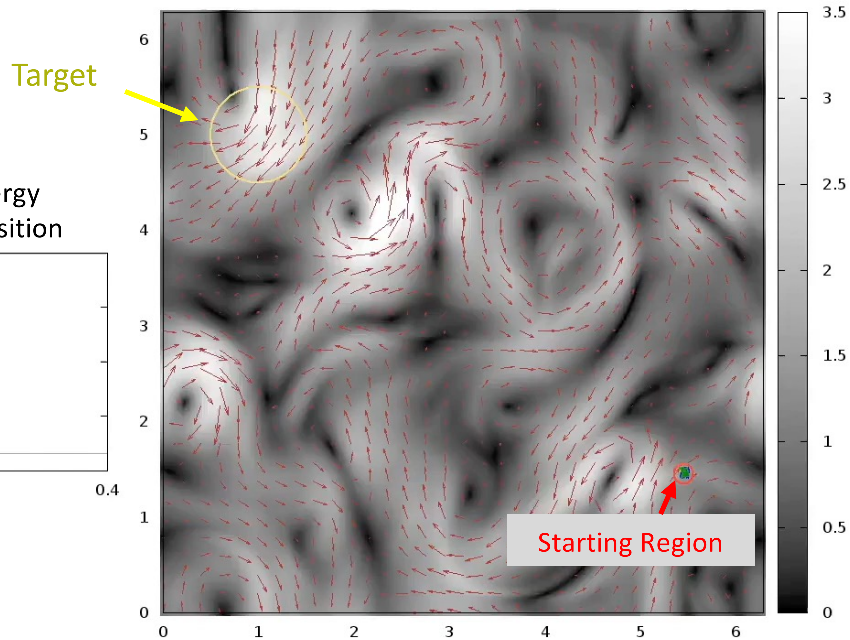
Total Reward





Flow kinetic energy
at the particle position

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



Reinforcement Learning (blue)

vs

Trivial Policy (green)

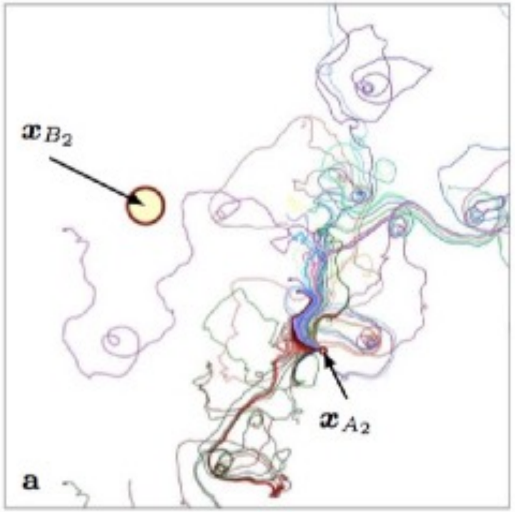
COMPARISON RL VS OPTIMAL NAVIGATION

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

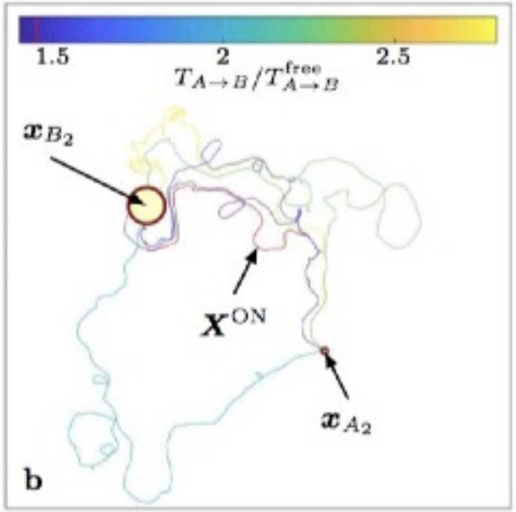
Time independent flow

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

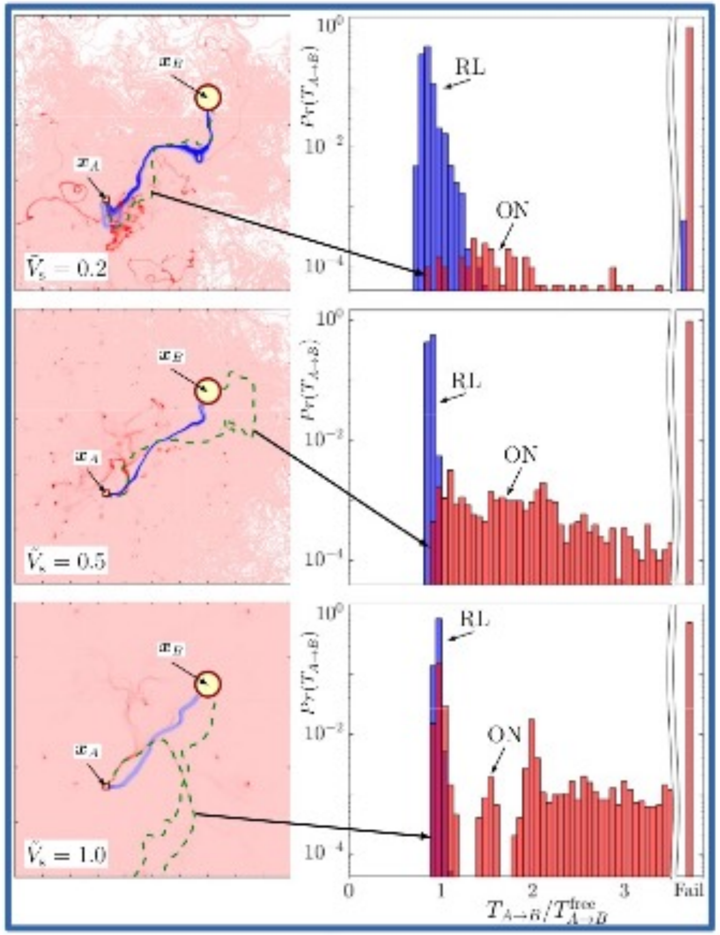
$$\dot{\theta}_t = A_{21}\sin^2\theta_t - A_{12}\cos^2\theta_t + (A_{11} - A_{22})\cos\theta_t \sin\theta_t\,,$$



1000 trials (all failures)



100k trials (10 successes)



WHAT WE HAVE:

- QUICK STOCHASTIC TOOL TO GENERATE REALISTIC 3D TRAJECTORIES OF TRACERS IN HOMOGENEOUS AND ISOTROPIC TURBULENCE, EASY TO GENERALISE FOR DIFFERENT APPLICATIONS

- VERY GOOD QUANTITATIVE AGREEMENT WITH MULTI-SCALE STATISTICAL PROPERTIES

WHAT WE MISS:

- UNDERSTADING OF ROBUSTNESS IN GENERALISING OUT-OF-SAMPLE:
EXTREME EVENTS, DIFFERENT REYNOLDS NUMBERS, DIFFERENT PARTICLES' PROPERTIES

- UNDERSTANDING SCALING PROPERTIES FOR TIME-TO-SOLUTION AT CHANGING IN-SAMPLE PROPERTIES, I.E. AT CHANGING DIMENSION OF THE TRAINING DATASET,
SETS OF HYPER-PARAMETERS, CNN ARCHITECTURES: GAN, DM, TRANSFORMERS

-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

Stéphane Mallat
Collège de France, Paris, France
Flatiron Institute, New York, USA

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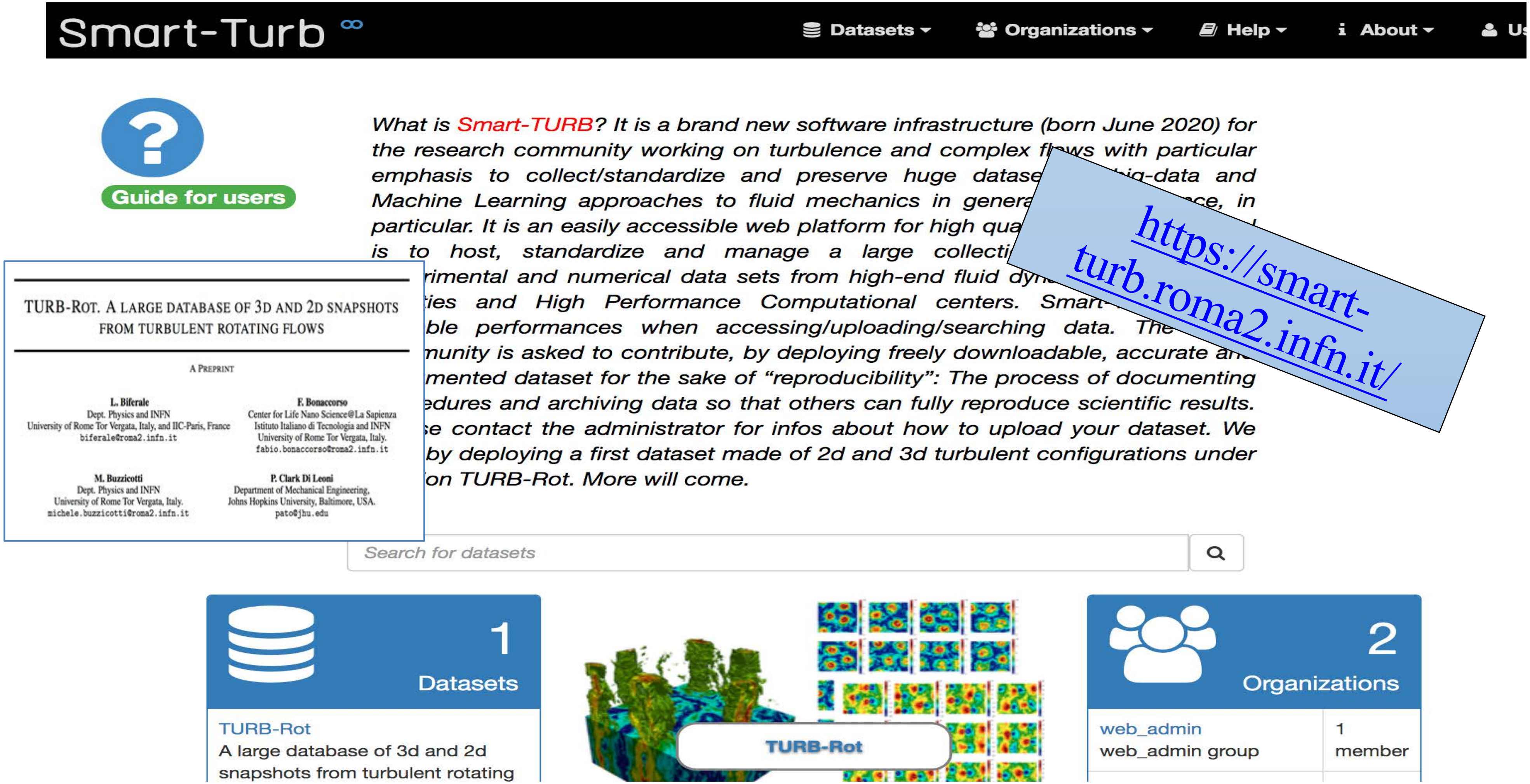
Smart-Turb
Datasets
Organizations
Help
About
Guide for users
What is Smart-TURB? It is a brand new software infrastructure (born June 2020) for the research community working on turbulence and complex flows with particular emphasis to collect/standardize and preserve huge datase
Machine Learning approaches 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
nunity 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.
e 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
L. Biferale
Dept. Physics and INFN
University of Rome Tor Vergata, Italy, and IIC-Paris, France
biferale@roma2.infn.it
F. Bonaccorso
Center for Life Nano Science@La Sapienza
Istituto Italiano di Tecnologia and INFN
University of Rome Tor Vergata, Italy.
fabio.bonaccorso@roma2.infn.it
M. Buzzicotti
Dept. Physics and INFN
University of Rome Tor Vergata, Italy.
michele.buzzicotti@roma2.infn.it
P. Clark Di Leoni
Department of Mechanical Engineering,
Johns Hopkins University, Baltimore, USA.
pato@jhu.edu
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1
Datasets
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A large database of 3d and 2d
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2
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