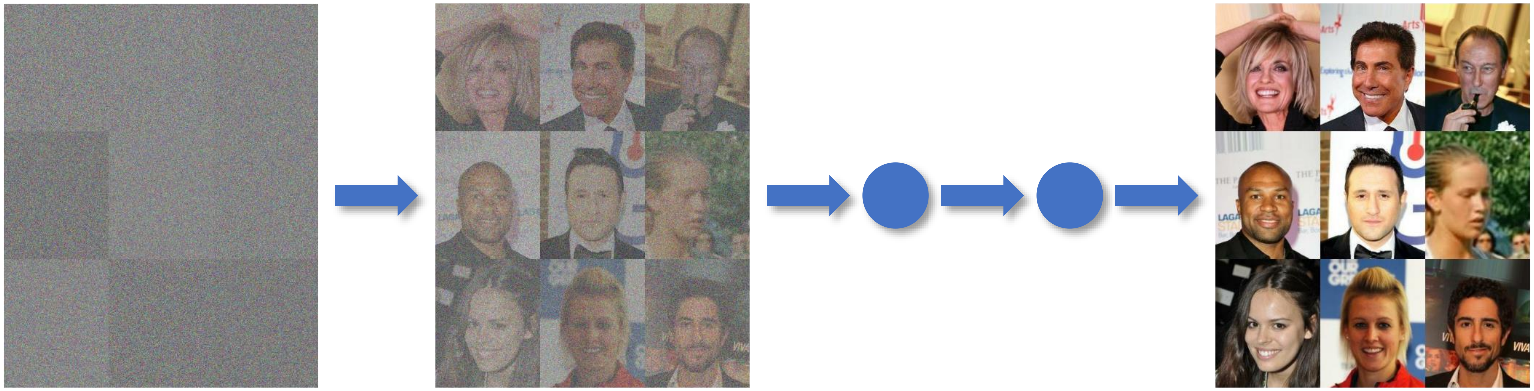


Generative Diffusion Models in Turbulence: Lagrangian data generation and Eulerian field reconstruction

T. Li, M. Buzzicotti, L. Biferale, A. Lanotte, F. Bonaccorso and M. Scarpolini

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

AQTIVATE WORKSHOP, 28th Feb. 2024, Berlin

1. Short introduction to Eulerian and Lagrangian Turbulence
2. Recap of Denoising Diffusion Models
3. Diffusion Models (DMs) for Lagrangian Turbulence Synthesis
4. Conditioning DMs for Eulerian Turbulence Reconstruction

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

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

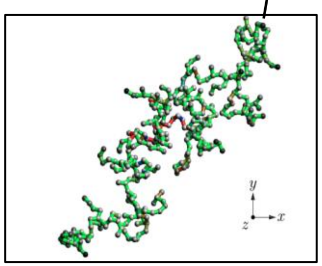
temperature

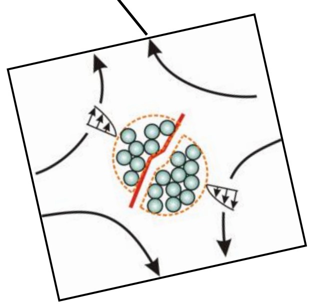
magnetic field

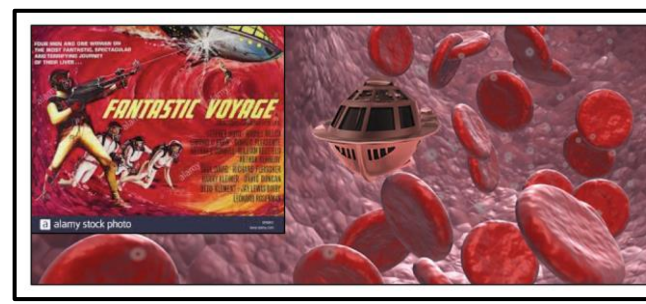
small active/passive
particles/droplets/bubbles/colloidal aggregates

LAGRANGIAN

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







COMPLEX FLUIDS & COMPLEX FLOWS

EULERIAN

$$\begin{cases} \partial_t v + v \cdot \partial_x v = -\partial_x p + \nu \partial^2 v \quad + f \\ \partial_x \cdot v = 0 \\ +b.c. \end{cases}$$

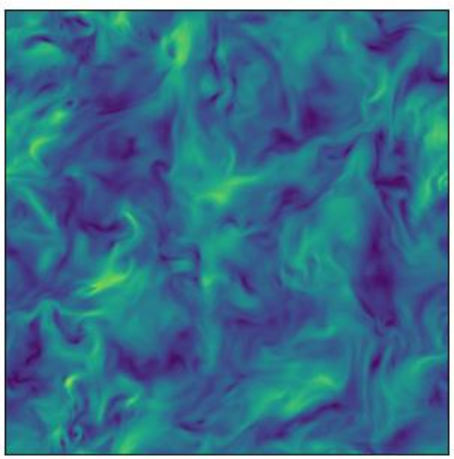
temperature

magnetic field

LAGRANGIAN

passive fluid tracers

$$\left\{ \dot{X}_i = v(X_i(t), t) \right.$$

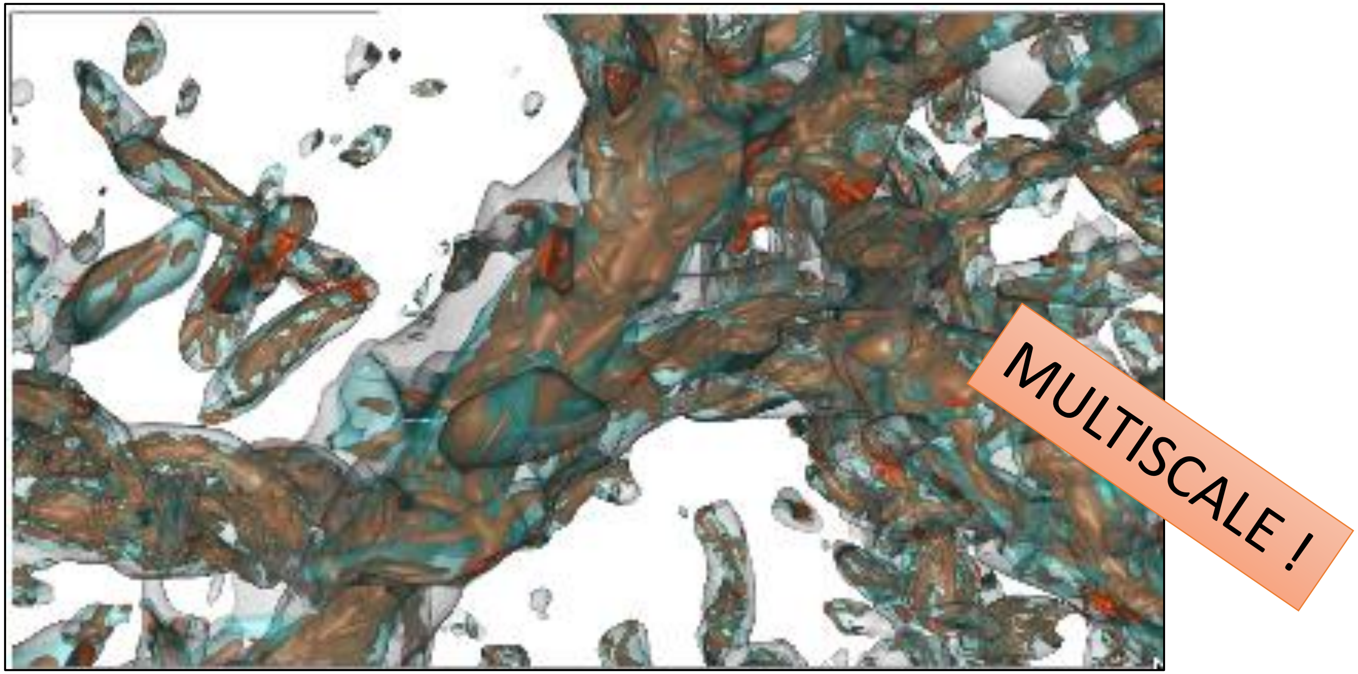


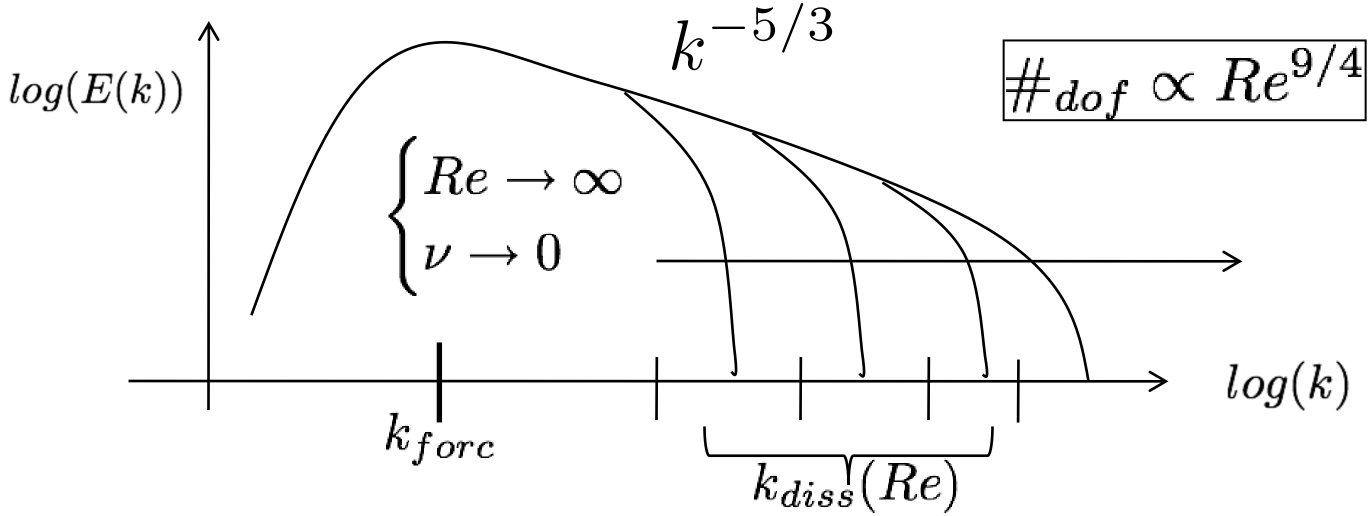
https://github.com/spectralDNS/spectralDNS

CONTROL PARAMETER:

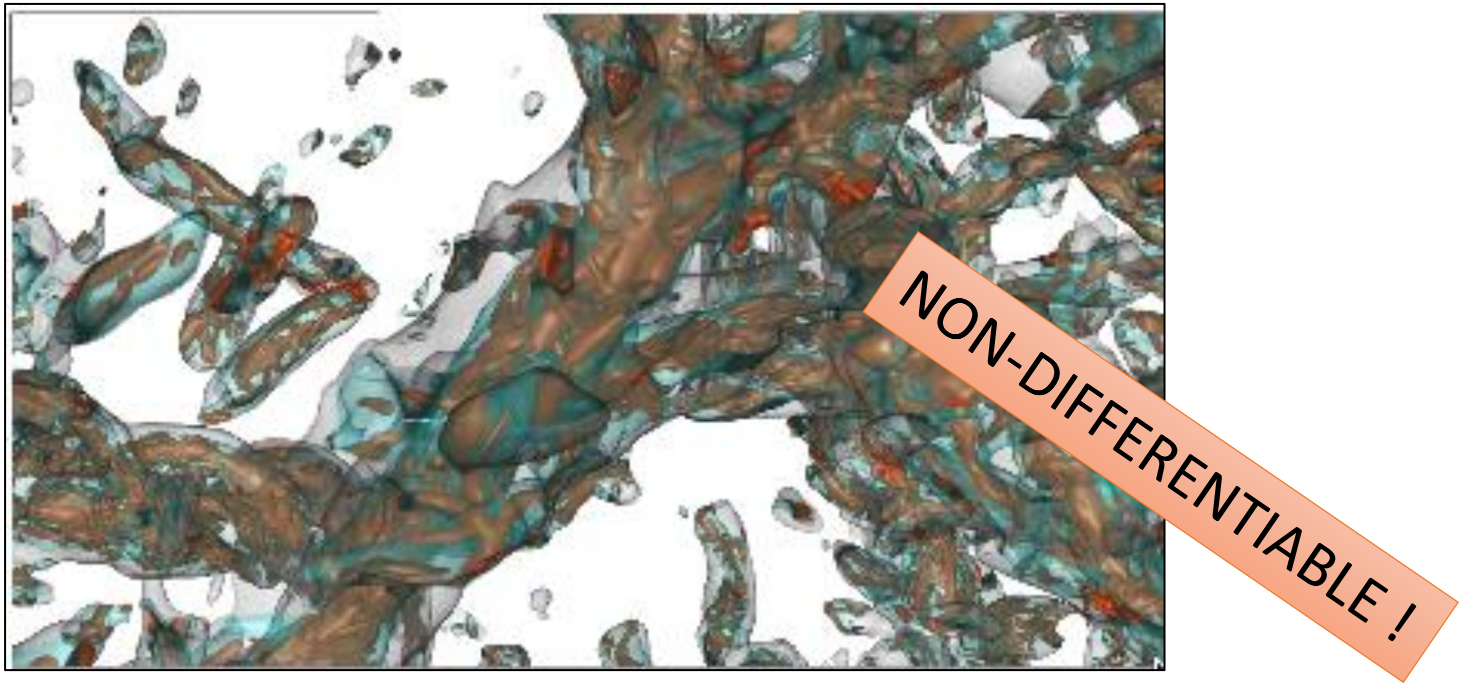
$$Re \sim \frac{v \partial_x v}{\nu \partial^2 v} \sim \frac{v_0 L_0}{\nu}$$

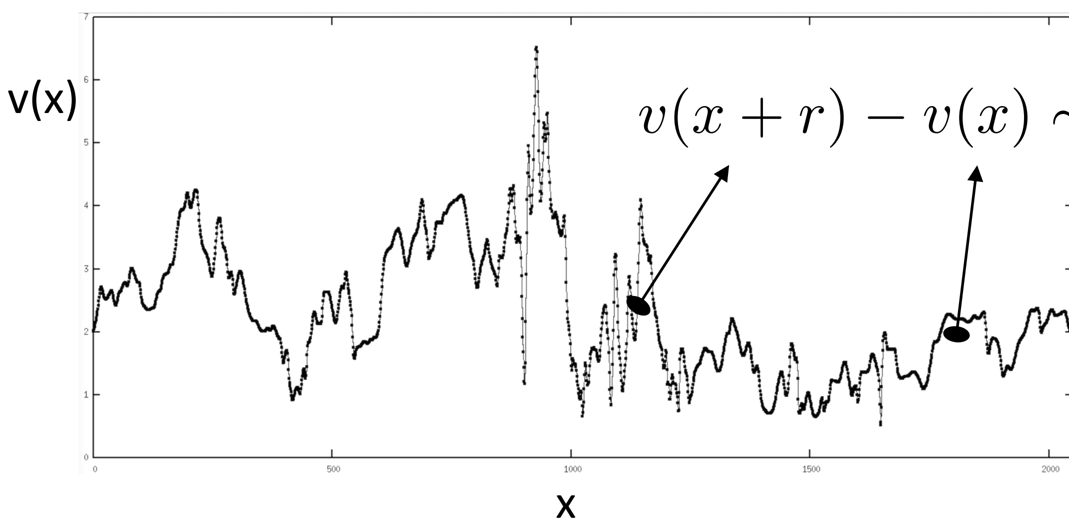
NAVIER-STOKES 3D





NAVIER-STOKES 3D

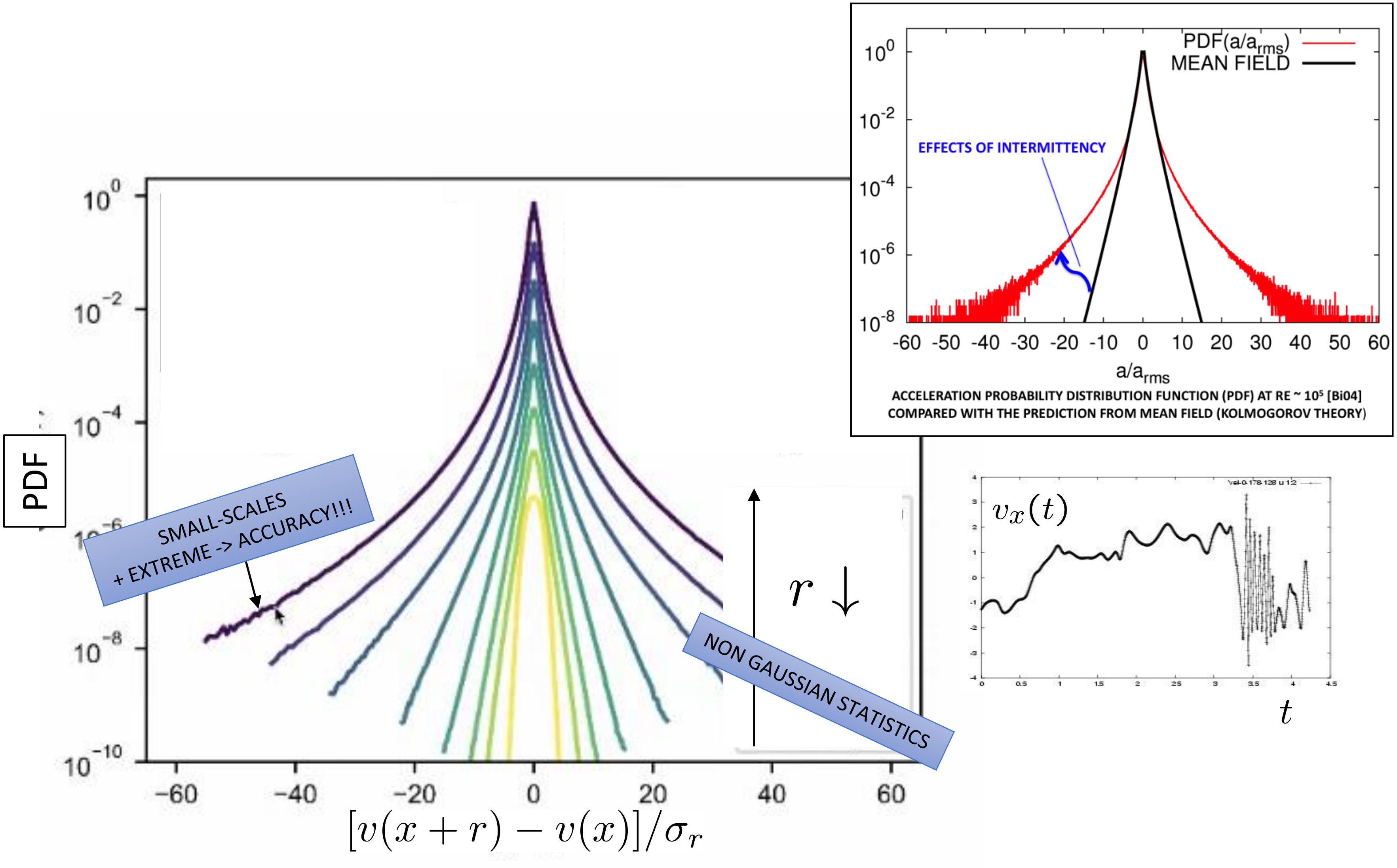




$$v(x+r) - v(x) \sim r^{1/3}$$

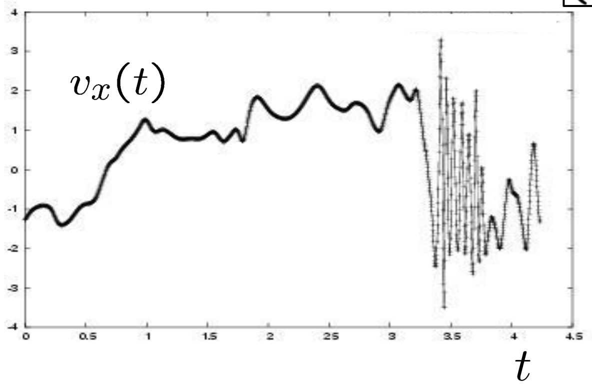
Holder continuos 1/3
non-differentiable!

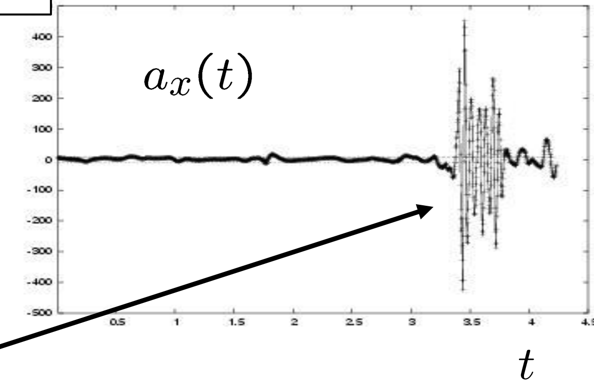
NAVIER-STOKES 3D



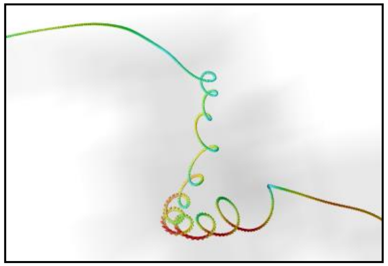
Bentkamp, L, Cr C. Lalescu, and M. Wilczek. "*Nature communications* 10.1 (2019): 1-8.

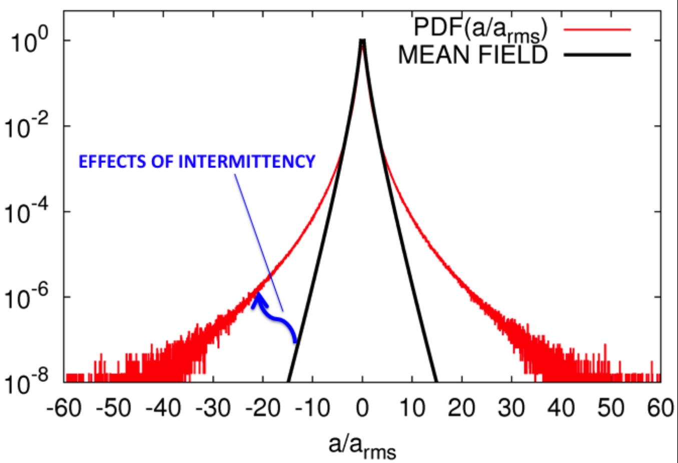
$$\begin{cases} \mathbf{a} = \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \nu \Delta \mathbf{u} + \mathbf{f} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$





EXTREME EVENTS



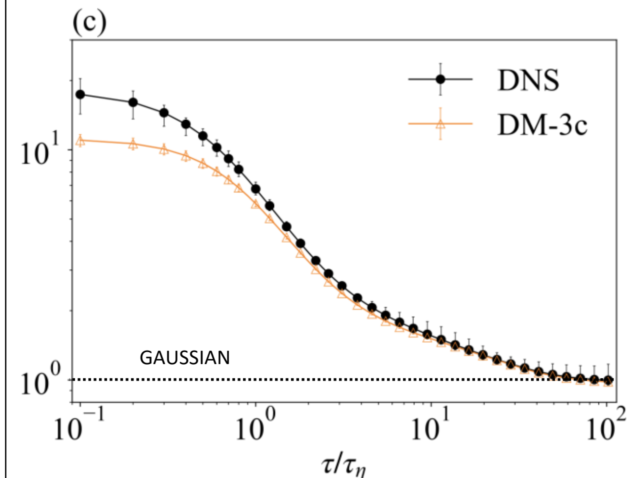


ACCELERATION PROBABILITY DISTRIBUTION FUNCTION (PDF) AT RE ~ 10^5 [Bi04] COMPARED WITH THE PREDICTION FROM MEAN FIELD (KOLMOGOROV THEORY)

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)



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

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

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

L Biferale, G Boffetta, A Celani, A Lanotte, F Toschi. Particle trapping in three-dimensional fully developed turbulence Physics of Fluids 17 (2), 021701 (2005)

COMPLEX FLUIDS & COMPLEX FLOWS

EULERIAN

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

temperature

m

ve

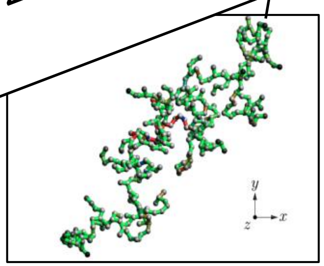
roplets/bubbles/colloidal aggregates

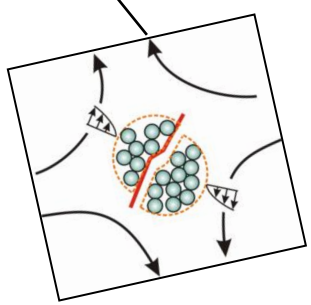
LAGRANGIAN

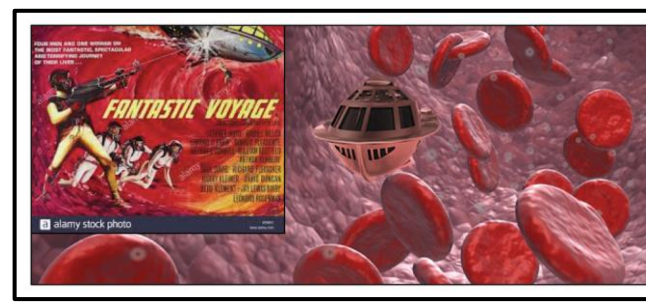
$$\begin{cases} \dot{X}_i = U_i \\ \dot{U}_i = \frac{v(X_i)-U_i}{\;} \end{cases}$$

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

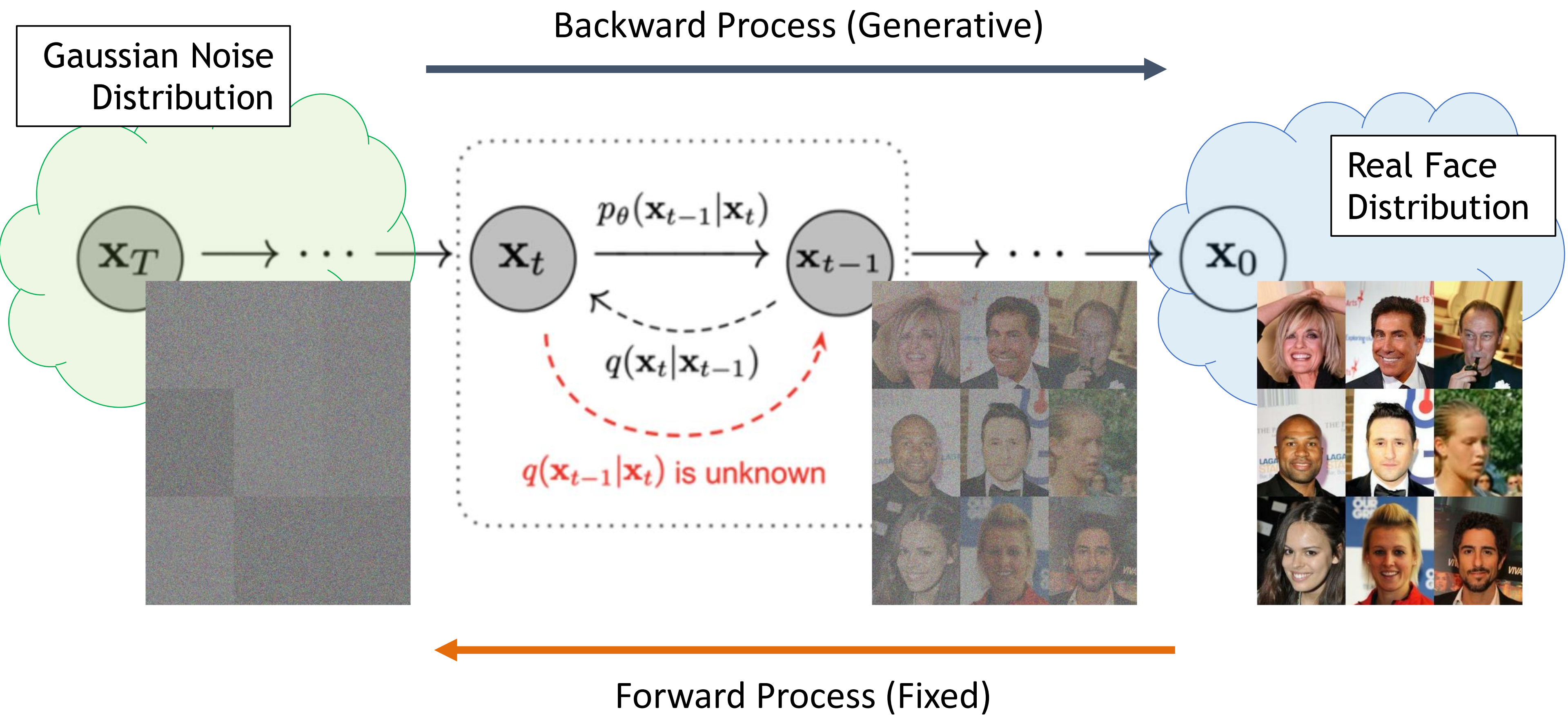
WE NEED QUANTITATIVE MODELS AND TOOLS TO MODEL!







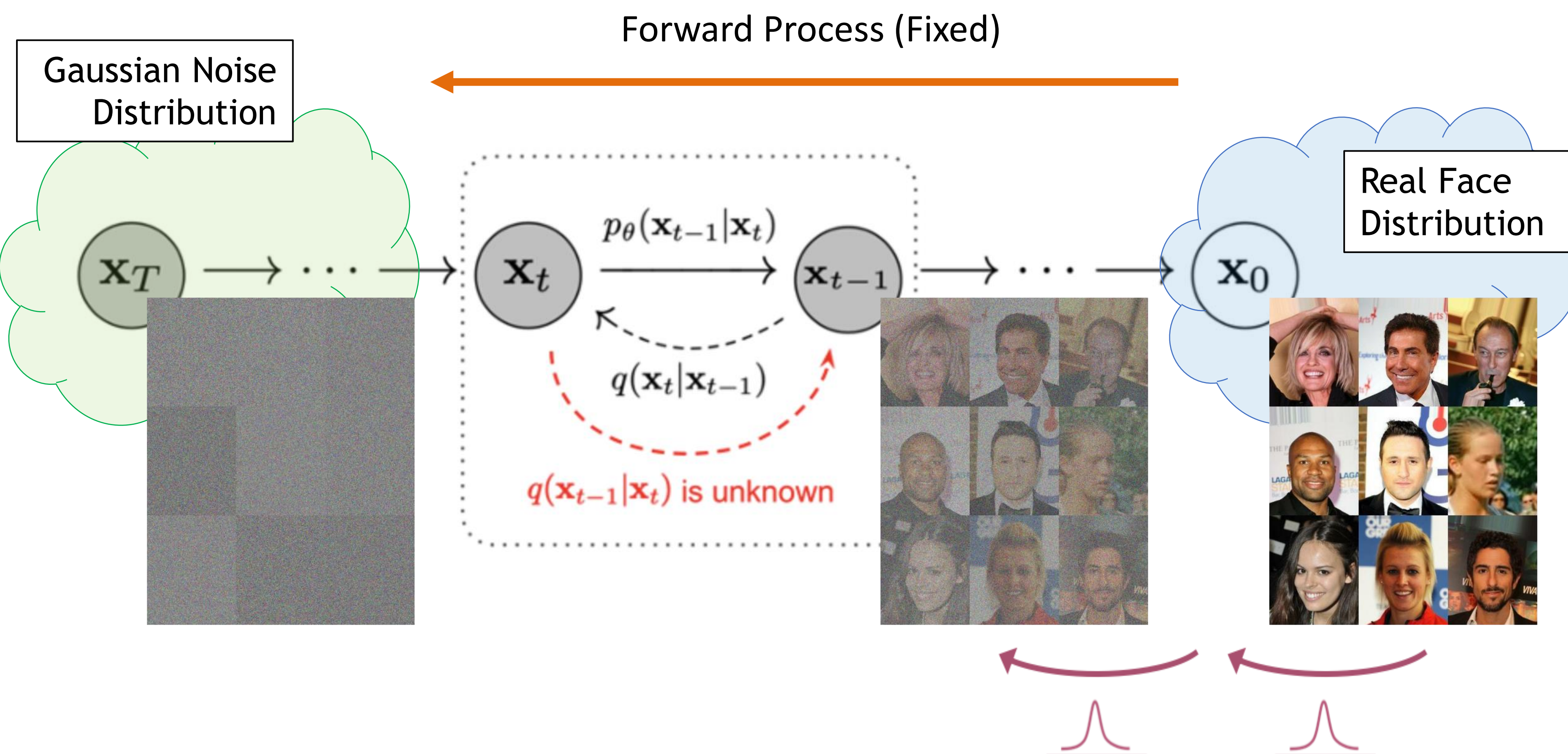
Denoising Diffusion Models



Learning to generate by denoising

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

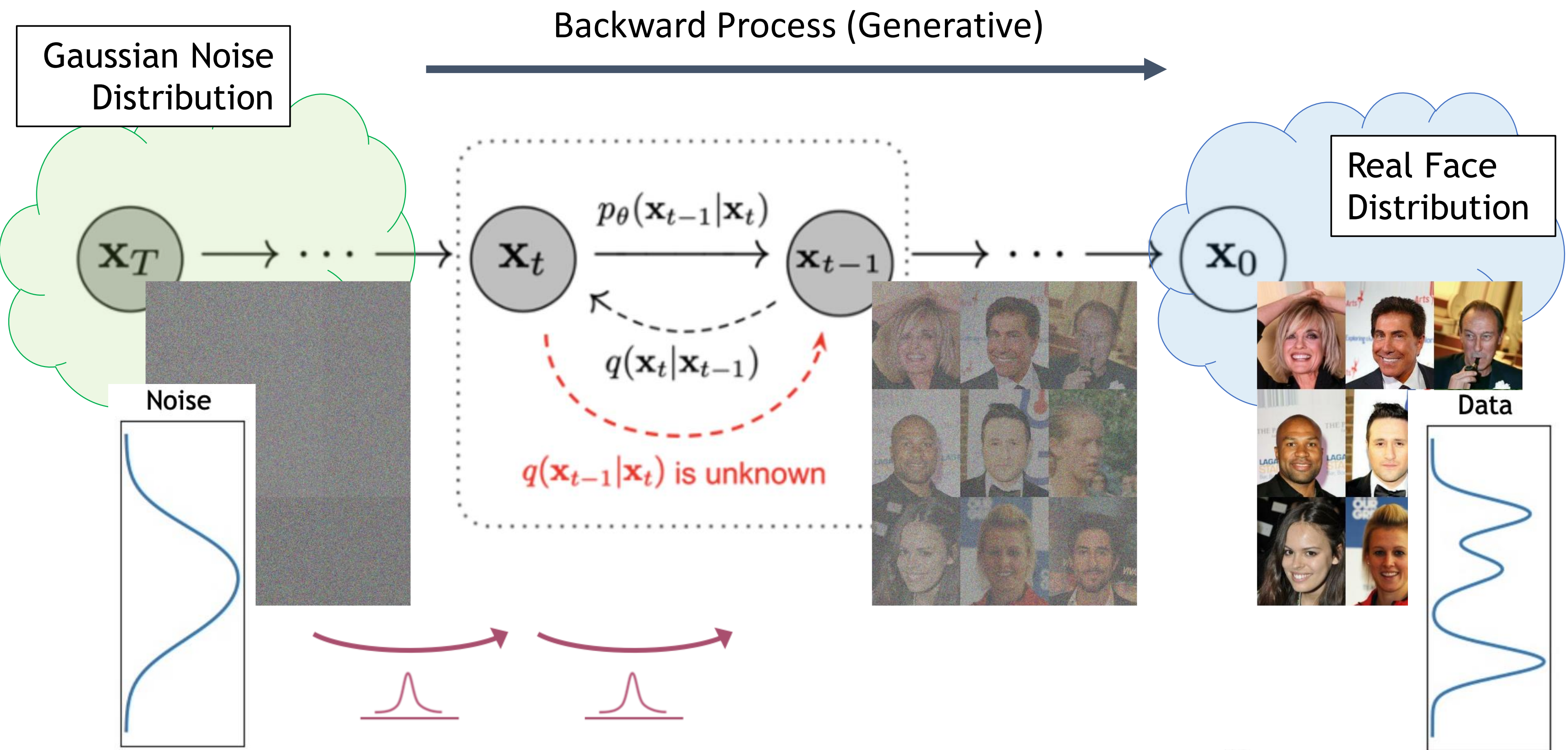
Forward Diffusion Process



The formal definition of the forward process in T steps:

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x_t}; \sqrt{1-\beta_t}\mathbf{x_{t-1}}, \beta_t\mathbf{I}) \quad \Rightarrow \quad q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})$$

Approx. Backward Diffusion Process



$$p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$$

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \underbrace{\mu_\theta(\mathbf{x}_t, t)}_{\text{Trainable network (U-net, Denoising Autoencoder)}}, \sigma_t^2\mathbf{I})$$

$$\Rightarrow \quad p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T)\prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$$

Learning the Backward Diffusion Process

Variational upper bound

$$\boxed{\mathbb{E}_{q(\mathbf{x}_0)}[-\log p_\theta(\mathbf{x}_0)]}$$

During training, the optimization involves **minimizing the cross entropy** between the ground truth distribution and the likelihood of the generated data

$$\mathbb{E}_{q(\mathbf{x}_0)}[..] = \int [..] q(\mathbf{x}_0) d\mathbf{x}_0 \qquad p_\theta(\mathbf{x}_0) = \int p_\theta(\mathbf{x}_{0:T}) d\mathbf{x}_{1:T} = \int p(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) d\mathbf{x}_{1:T}$$

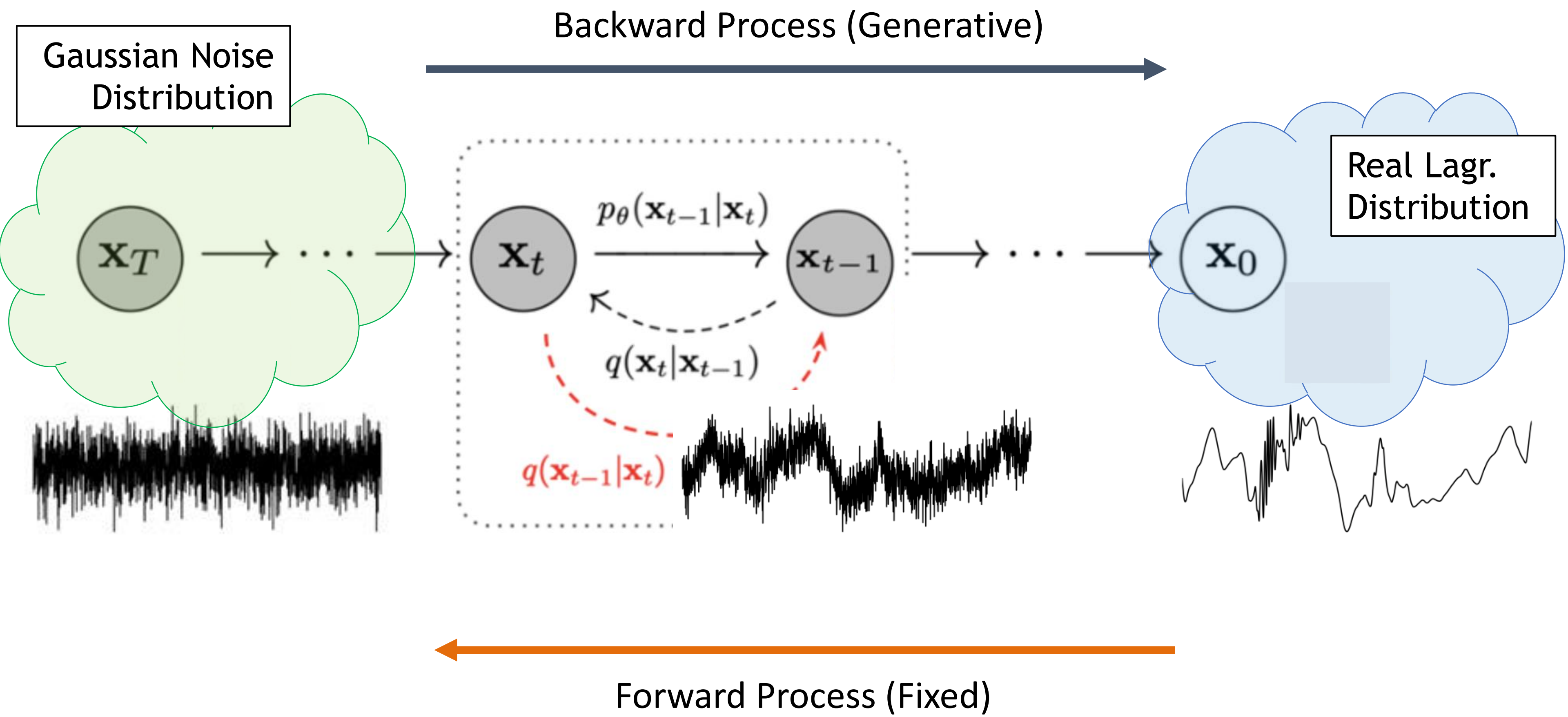
For training, we can form **variational upper bound** that is commonly used for training variational autoencoders:

$$\mathbb{E}_{q(\mathbf{x}_0)}[-\log p_\theta(\mathbf{x}_0)] \leq \mathbb{E}_{q(\mathbf{x}_0)q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] =: L$$

Sohl-Dickstein et al. ICML 2015 (Appendix B for all details) show that:

$$L = \mathbb{E}_q\left[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0)||p(\mathbf{x}_T))}_{L_T} + \sum_{t>1} \underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)||p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{- \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0}\right]$$

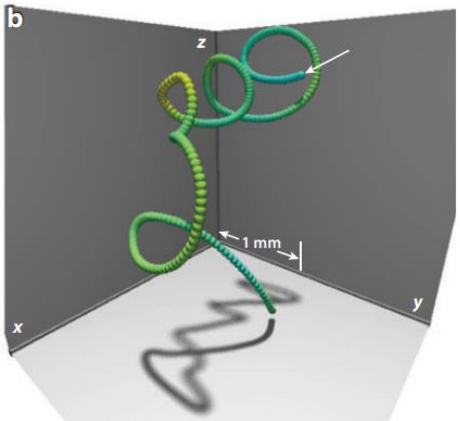
Diffusion Models for Lagrangian Turbulence



Learning to generate by denoising

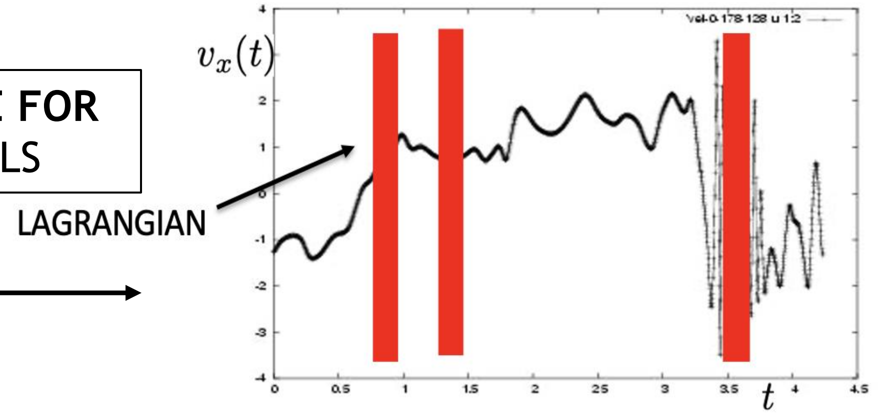
T. Li, L. Biferale, F. Bonaccorso, M. Scarpolini and M. Buzzicotti.
Synthetic Lagrangian Turbulence by Generative Diffusion Models.
arXiv:2307.08529 (2023) – Accepted by Nature Machine Intelligence

STOCHASTIC MODELS FOR LAGRANGIAN TURBULENCE: WHY?



LIMITATION OF ACQUIRING DATA FROM NUMERICAL SIMULATIONS AND EXPERIMENTS

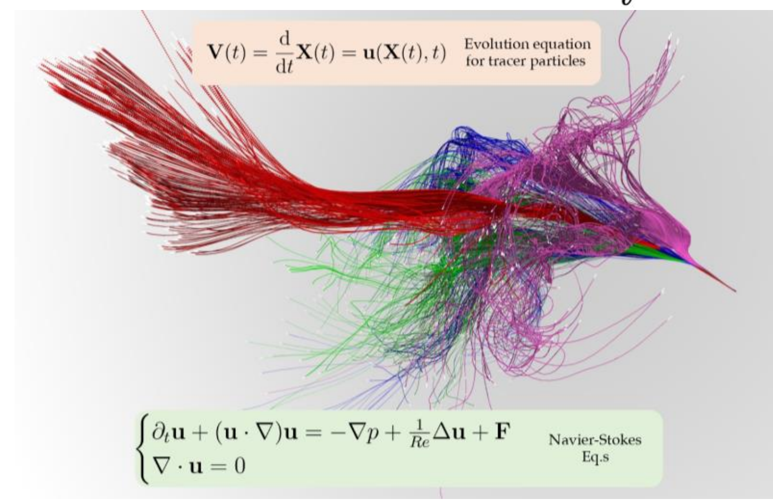
GENERATION OF LARGE SYNTHETIC DATA-BASE FOR TESTING DOWNSTREAM APPLICATIONS/MODELS



DATA ASSIMILATION/INPAINTING FROM MISSING FIELD/EXPERIMENTAL OBSERVATION

CLASSIFICATION/INFERRAL OF MISSING/INTERNAL PROPERTIES:

(I) INERTIA
(II) SHAPE
(III) ACTIVE DEGREES OF FREEDOM
(IV) ….



~30 years of modeling experience

Sawford, B. L. Reynolds number effects in Lagrangian stochastic models of turbulent dispersion. Phys. Fluids A: Fluid Dyn. 3, 1577–1586 (1991).

Wilson, J. D. & Sawford, B. L. Review of lagrangian stochastic models for trajectories in the turbulent atmosphere. Boundary-layer meteorology 78, 191–210 (1996).

Biferale, L., Boffetta, G., Celani, A., Crisanti, A. & Vulpiani, A. Mimicking a turbulent signal: Sequential multiaffine processes. Physical Review E 57, R6261 (1998).

Arneodo, A., Bacry, E. & Muzy, J.-F. Random cascades on wavelet dyadic trees. Journal of Mathematical Physics 39, 4142–4164 (1998).

Lamorgese, A., Pope, S. B., Yeung, P. & Sawford, B. L. A conditionally cubic-gaussian stochastic lagrangian model for acceleration in isotropic turbulence. Journal of Fluid Mechanics 582, 423–448 (2007).

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).

Minier, J.-P., Chibbaro, S. & Pope, S. B. Guidelines for the formulation of lagrangian stochastic models for particle simulations of single-phase and dispersed two-phase turbulent flows. Physics of Fluids 26, 113303 (2014).

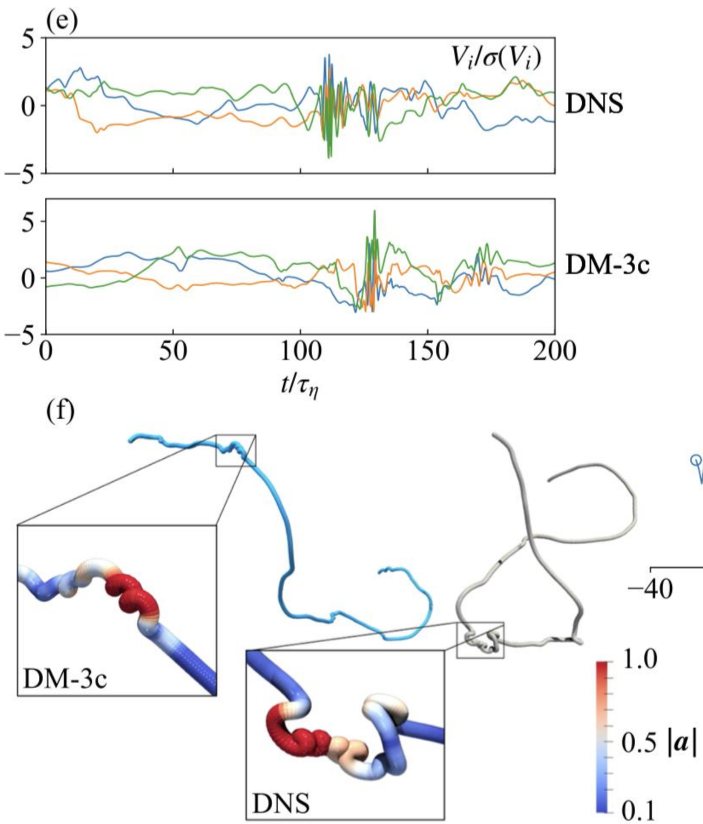
Chevillard, L., Garban, C., Rhodes, R. & Vargas, V. On a skewed and multifractal unidimensional random field, as a probabilistic representation of kolmogorov’s views on turbulence. In Annales Henri Poincaré, vol. 20, 3693–3741 (Springer, 2019).

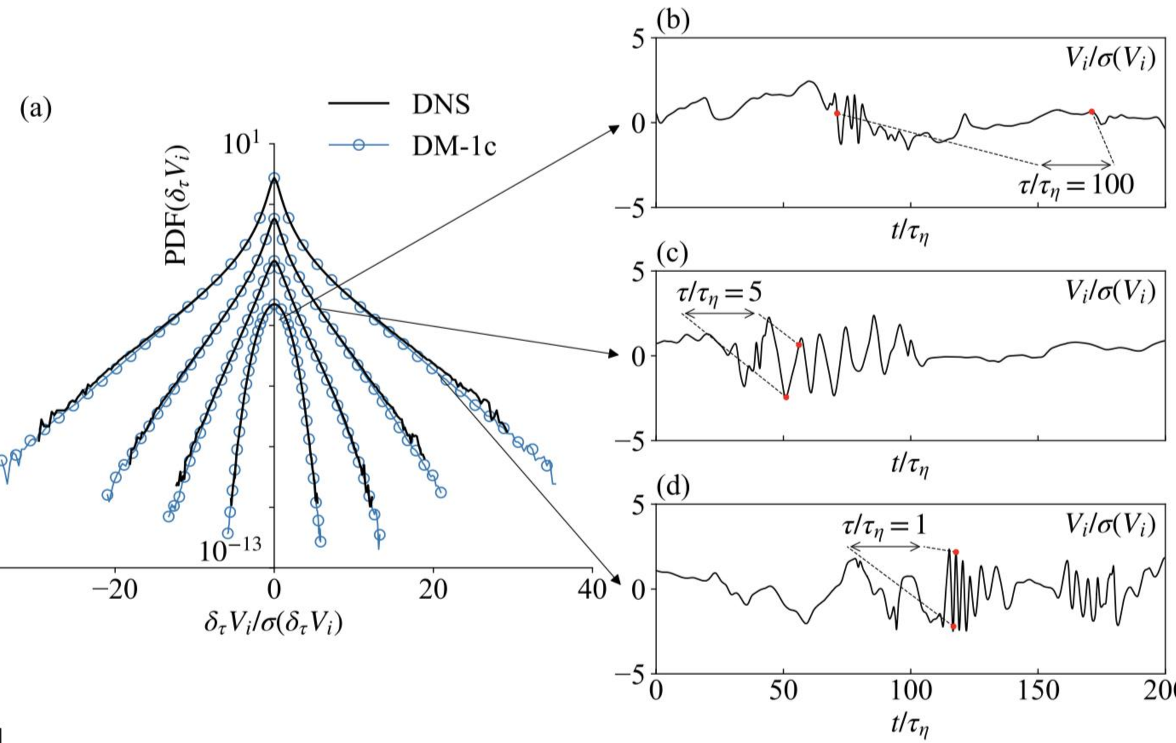
Viggiano, B. et al. Modelling lagrangian velocity and acceleration in turbulent flows as infinitely differentiable stochastic processes. Journal of Fluid Mechanics 900, A27 (2020).

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).

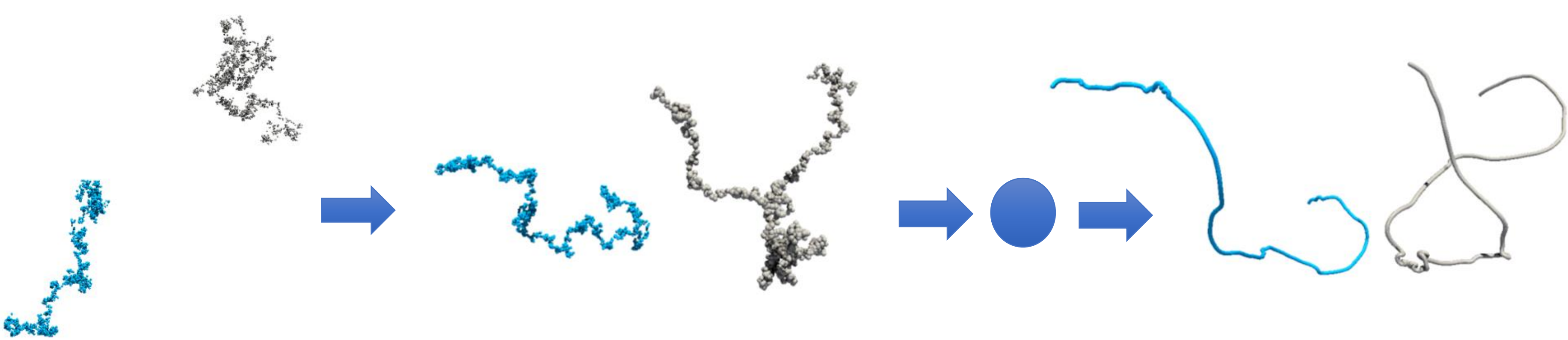
$$\delta_\tau V_i(t) = V_i(t+\tau) - V_i(t),$$





DM-1c: generate 1 velocity comp. (isotropic)

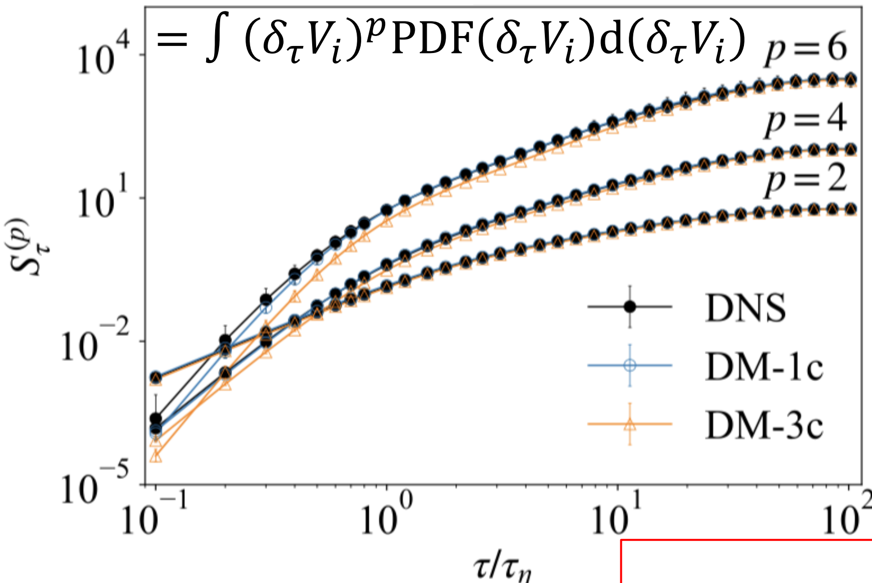
DM-3c: generate 3 velocity comps.



LAGRANGIAN STRUCTURE FUNCTIONS

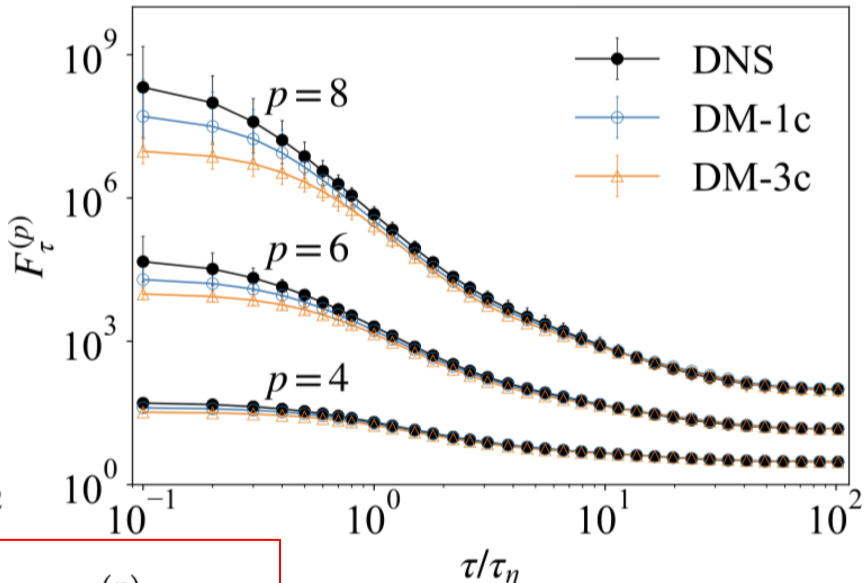
$$S_\tau^{(p)} = \langle (\delta_\tau V_i)^p \rangle$$

$$= \int (\delta_\tau V_i)^p \mathrm{PDF}(\delta_\tau V_i) \mathrm{d}(\delta_\tau V_i)$$

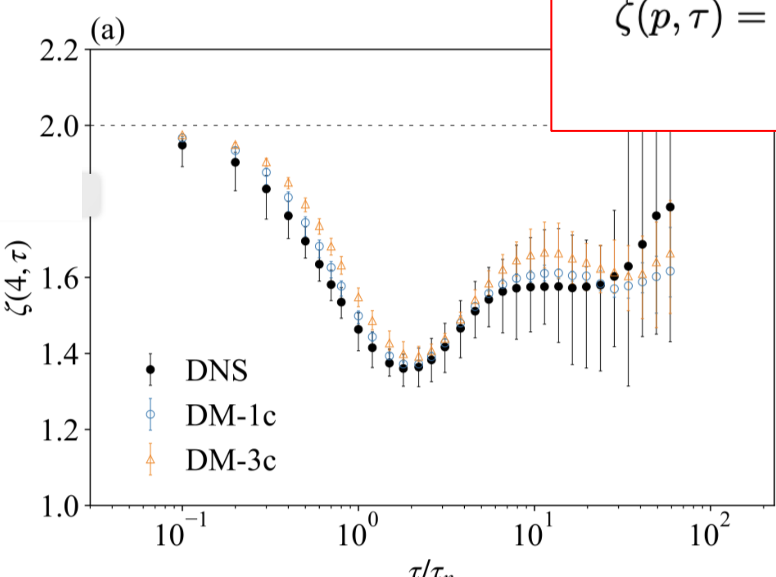


GENERALIZED FLATNESS

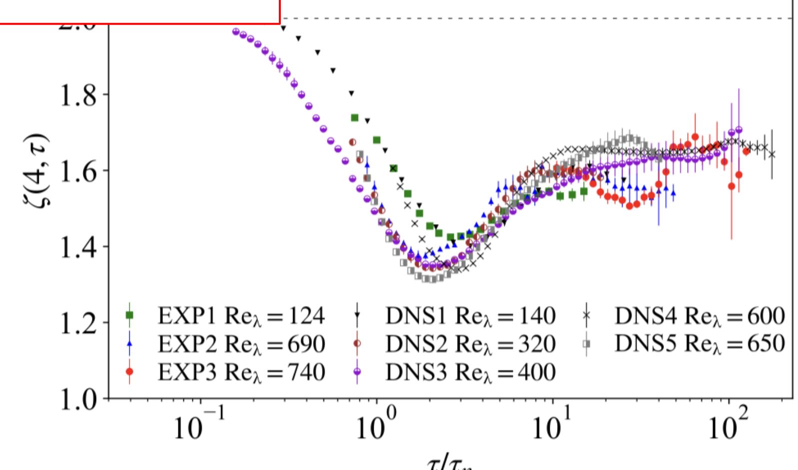
$$F_\tau^{(p)} = S_\tau^{(p)} / [S_\tau^{(2)}]^{p/2}.$$



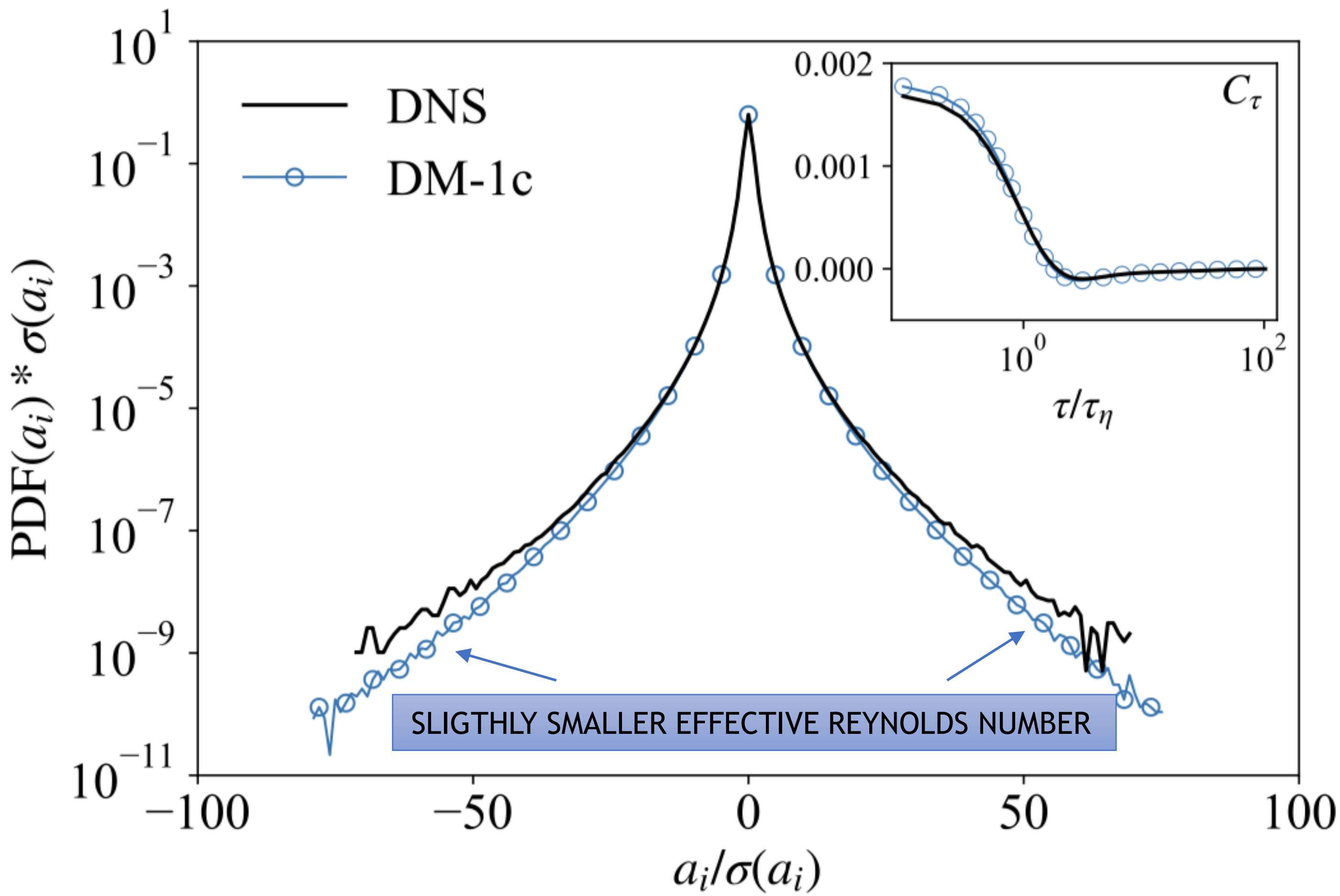
$$\zeta(p,\tau) = \frac{d \log S_\tau^{(p)}}{d \log S_\tau^{(2)}}.$$

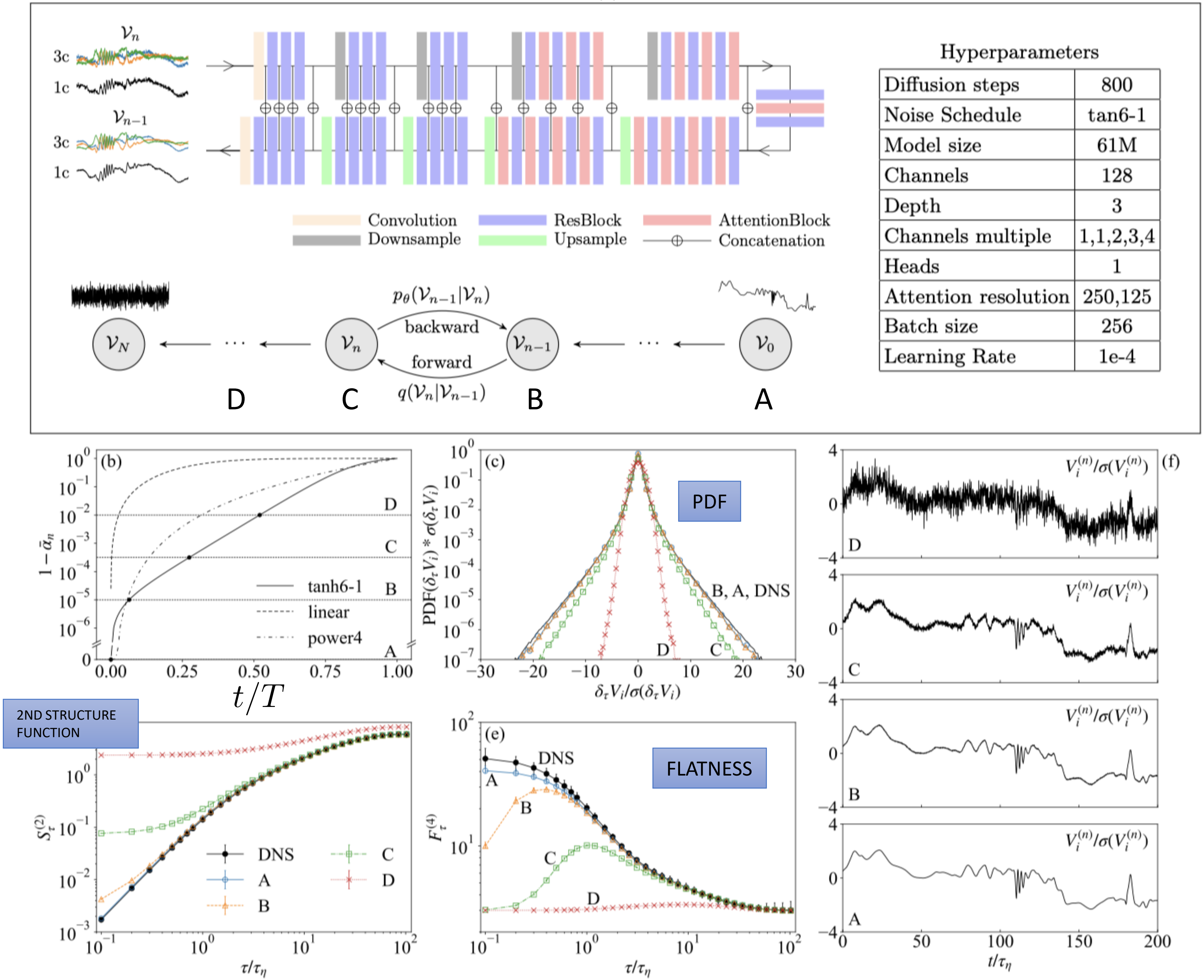


A. Arnèodo et al PRL 2008



ACCELERATION PDF

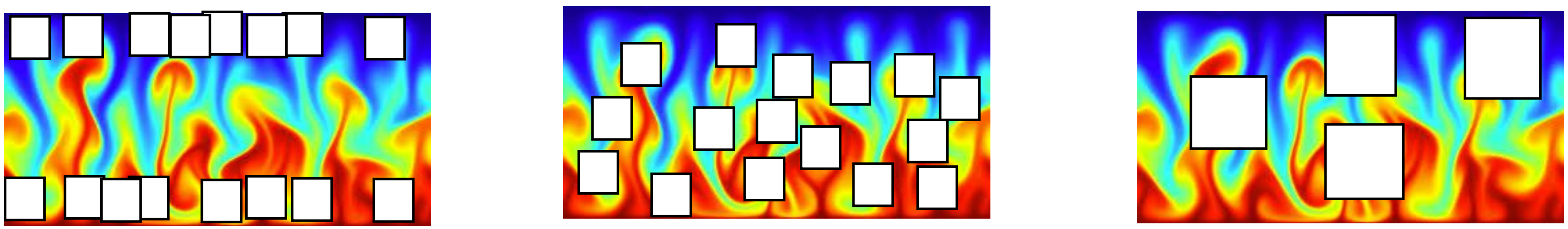



Hyperparameters
Diffusion steps 800
Noise Schedule tan6-1
Model size 61M
Channels 128
Depth 3
Channels multiple 1,1,2,3,4
Heads 1
Attention resolution 250,125
Batch size 256
Learning Rate 1e-4
Convolution
Downsample
ResBlock
Upsample
AttentionBlock
Concatenation
backward
forward
D
C
B
A
PDF
2ND STRUCTURE FUNCTION
FLATNESS
tanh6-1
linear
power4
B, A, DNS
DNS

1. RECONSTRUCTION OF MISSING INFORMATION (INPAINTING – SUPER RESOLUTION)
2. FEATURES RANKING: QUALITY AND QUANTITY OF DATA

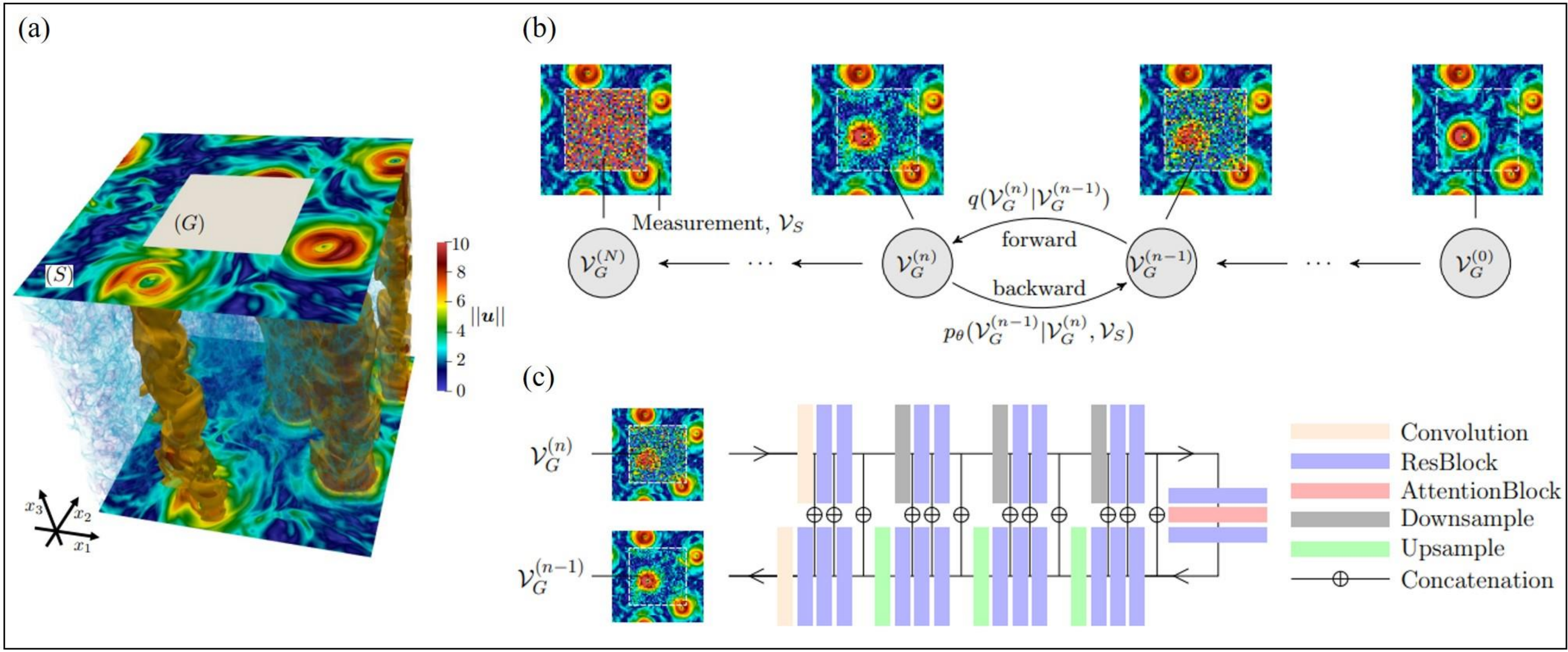
- IS IT BETTER TO INPUT SPATIAL OR TEMPORAL DATA?
- HOW MANY DATA/VARIABLES YOU NEED TO SUPPLY FOR PERFECT RECONSTRUCTION (SYNCHRONIZATION-TO-DATA)?
- CAN YOU GUESS VELOCITY FIELDS BY MEASURING ONLY TEMPERATURE AND/OR VICEVERSA?
- IS IT BETTER TO PROVIDE INFORMATION FROM BOUNDARIES OR BULK?
- FROM LARGE 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



Saharia, C., Chan, W., Chang, H., Lee, C., Ho, J., Salimans, T., ... & Norouzi, M. (2022, July). Palette: Image-to-image diffusion models. In *ACM SIGGRAPH 2022 Conference Proceedings* (pp. 1-10).

Conditional DM: Palette

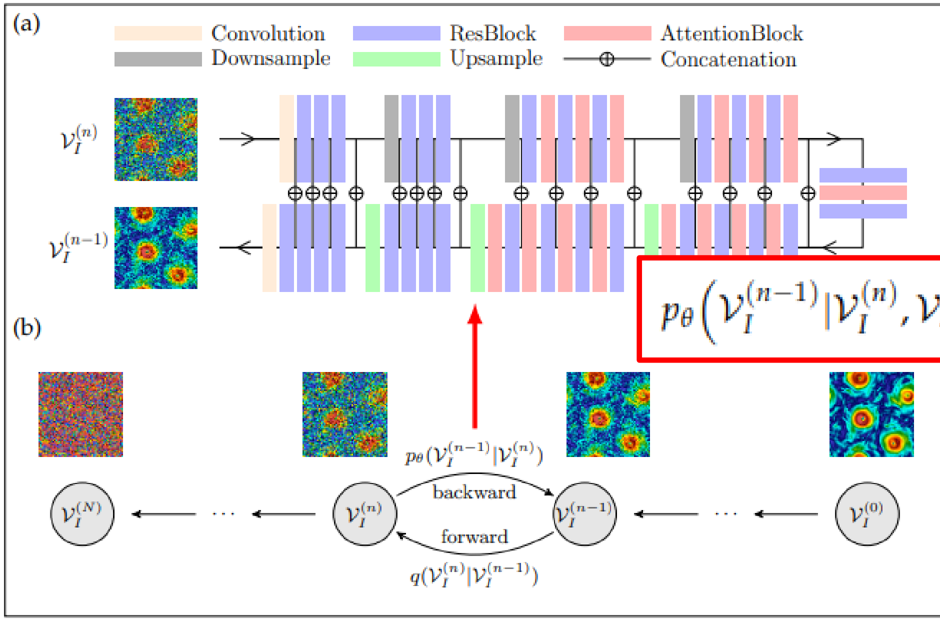


forward & backward processes

$$q(\mathcal{V}_G^{(1:N)}|\mathcal{V}_G^{(0)}) := \prod_{n=1}^{N} q(\mathcal{V}_G^{(n)}|\mathcal{V}_G^{(n-1)})$$

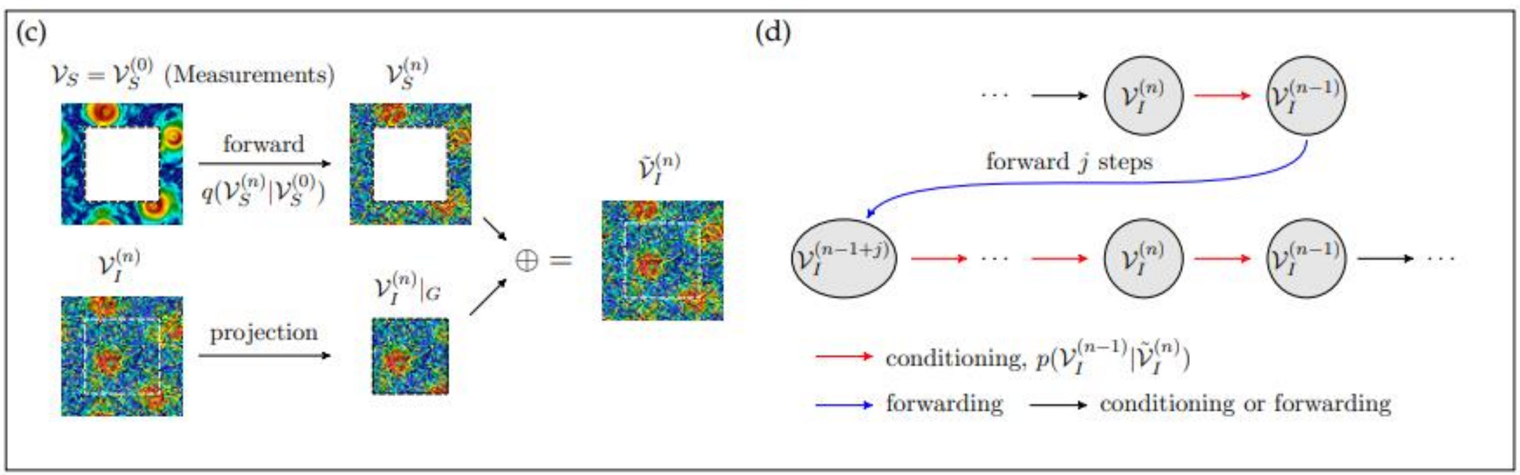
$$p_\theta(\mathcal{V}_G^{(0)}|\mathcal{V}_S) = p(\mathcal{V}_G^{(N)}) \prod_{n=1}^{N} p_\theta(\mathcal{V}_G^{(n-1)}|\mathcal{V}_G^{(n)}, \mathcal{V}_S)$$

Reconstruction with unconditional DM: RePaint



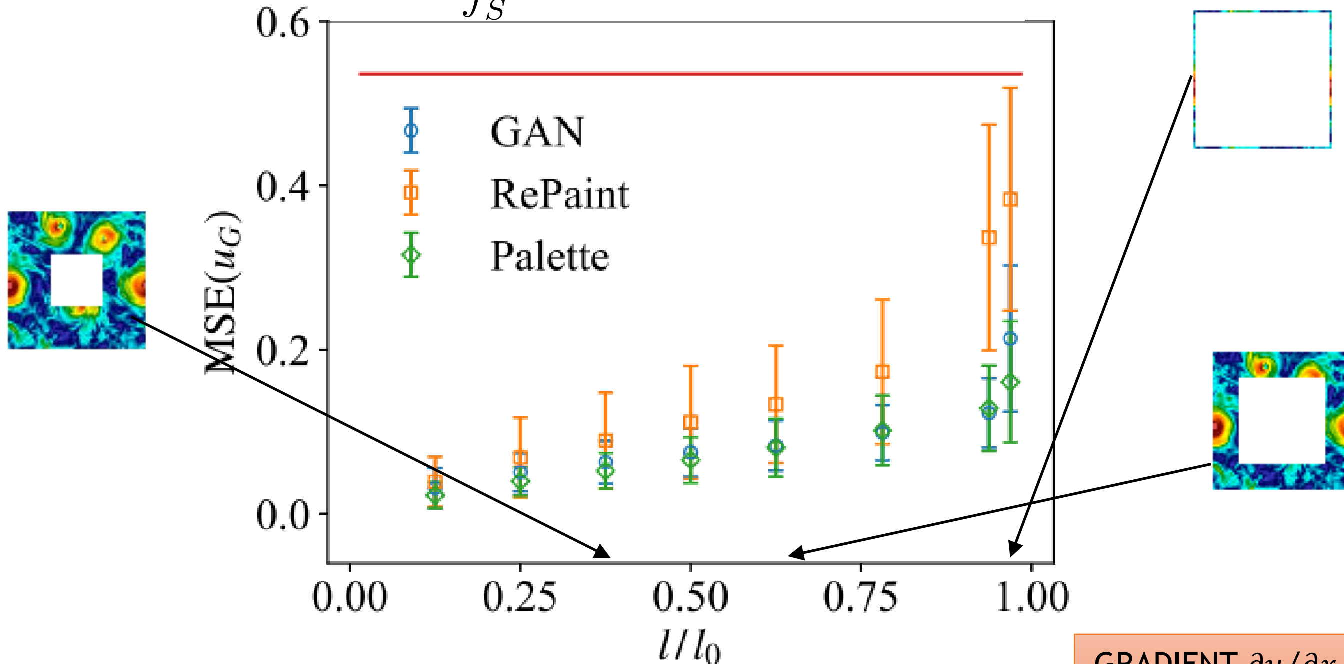
Conditioning heuristics:

$$\boxed{p_\theta\left(\mathcal{V}_I^{(n-1)}|\mathcal{V}_I^{(n)}, \mathcal{V}_S\right) \approx p_\theta\left(\mathcal{V}_I^{(n-1)}|\tilde{\mathcal{V}}_I^{(n)}\right) \quad \text{where} \quad \tilde{\mathcal{V}}_I^{(n)} = \mathcal{V}_I^{(n)}|_G \oplus \mathcal{V}_S^{(n)}.}$$

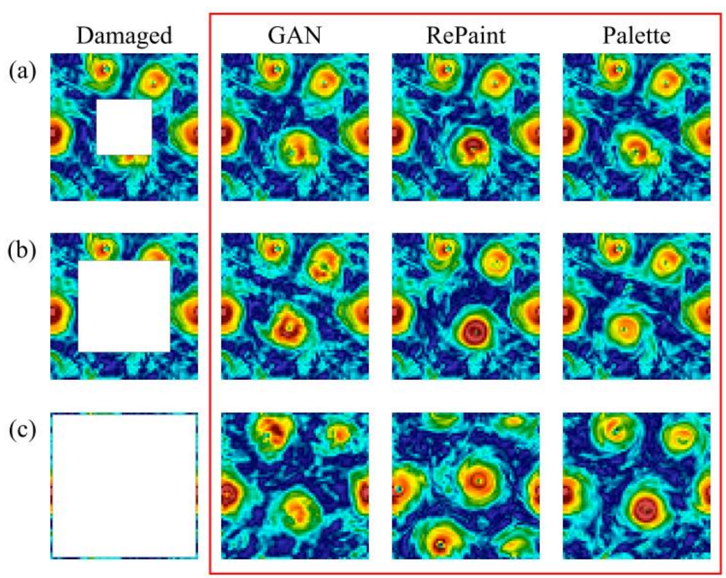


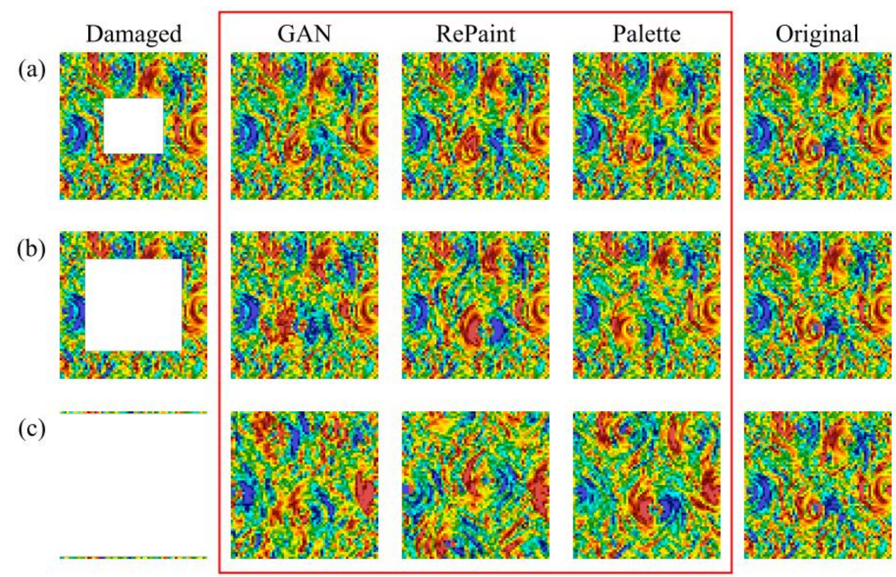
Lugmayr et al. Repaint: Inpainting using denoising diffusion probabilistic models. In Proceedings of the Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, 2022, pp. 11461–11471

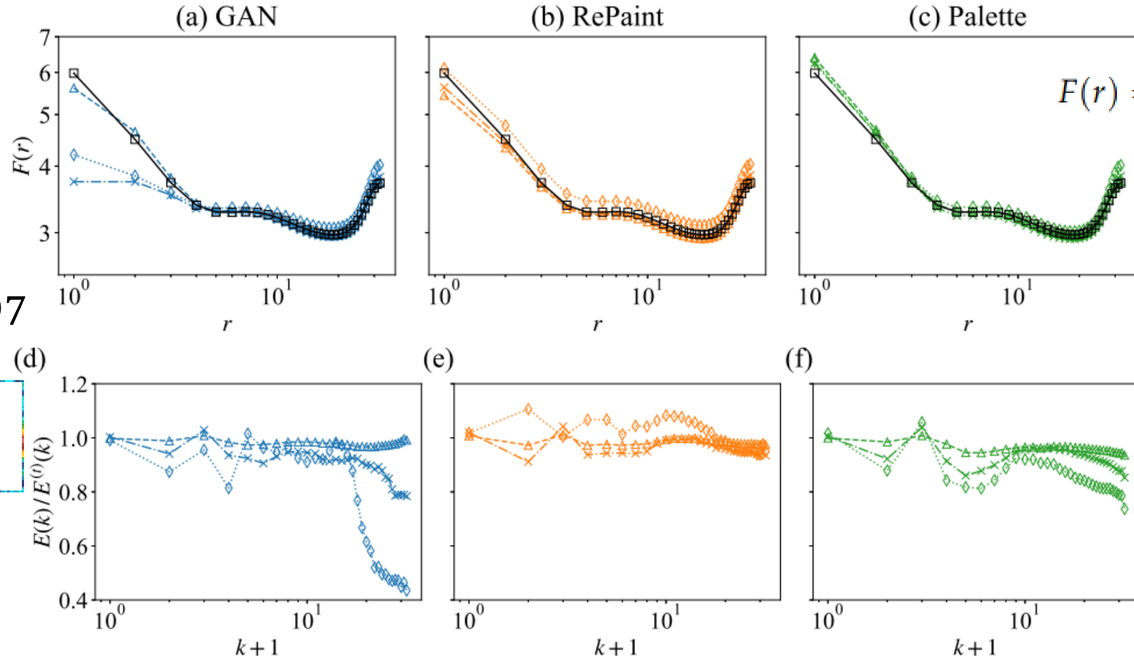
$$\mathcal{L}_G = \langle \int_S d\mathbf{x}(u_{true}(\mathbf{x}) - u_{pred}(\mathbf{x}, \theta))^2 \rangle$$



GRADIENT $\partial u/\partial x$

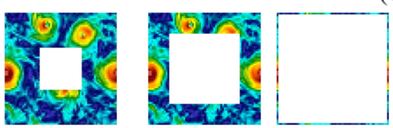


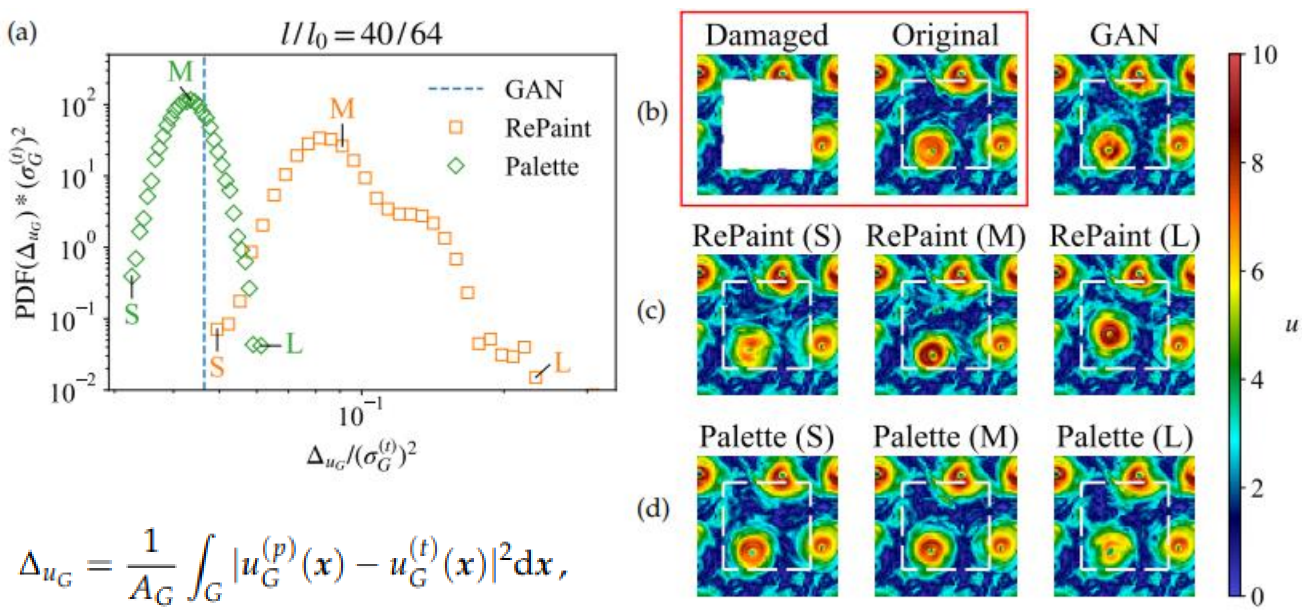




$$F(r) = \langle(\delta_r u)^4\rangle / \langle(\delta_r u)^2\rangle^2$$

$$l/l_0 = 0.38, 0.63, 0.97$$





$$\Delta_{u_G} = \frac{1}{A_G} \int_G |u_G^{(p)}(\boldsymbol{x}) - u_G^{(t)}(\boldsymbol{x})|^2 \mathrm{d}\boldsymbol{x},$$

WHAT WE HAVE:

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

- IMPRESSIVE QUANTITATIVE AGREEMENT WITH MULTI-SCALE STATISTICAL PROPERTIES

- DEFINE BECHMARKS AND CHALLENGES WITH HIGH QUALITY AND QUANTITY OF DATA AND WITH MULTI-SCALE MULTI-TIME BENCHMARKS

WHAT WE MISS:

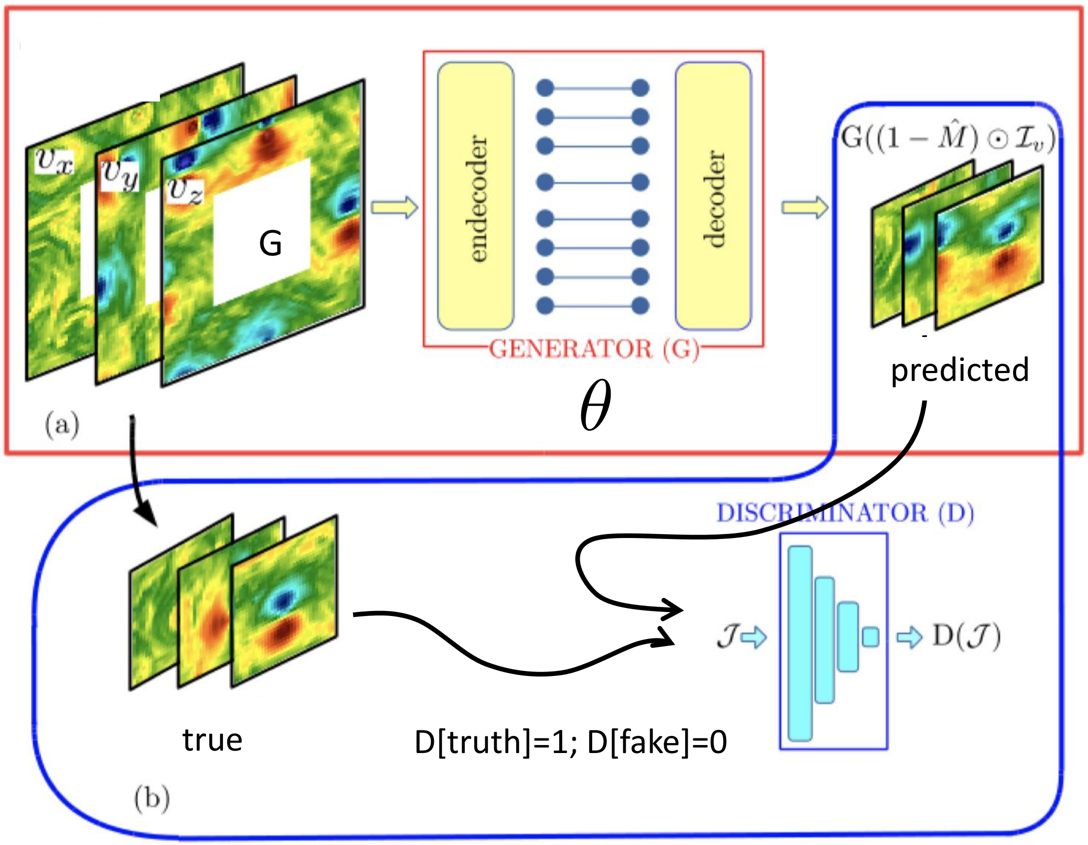
- UNDERSTADING OF ROBUSTNESS IN GENERALISING OUT-OF-SAMPLE:
EXTREME EVENTS, DIFFERENT REYNOLDS NUMBERS, DIFFERENT PARTICLES' PROPERTIES

- 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

All codes can be found in: https://github.com/SmartTURB

GENERATIVE ADVERSARIAL NETWORK: CONTEXT ENCODER (ACTOR-CRITIC)



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

MINIMIZE:

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

$$\mathcal{L}_{adv} = \log\left(1 - D\left(u_{\text{pred}}\right)\right).$$

$$\mathcal{L}_{TOT} = \mathcal{L}_G + \lambda \mathcal{L}_{ADV}$$

MAXIMIZE:

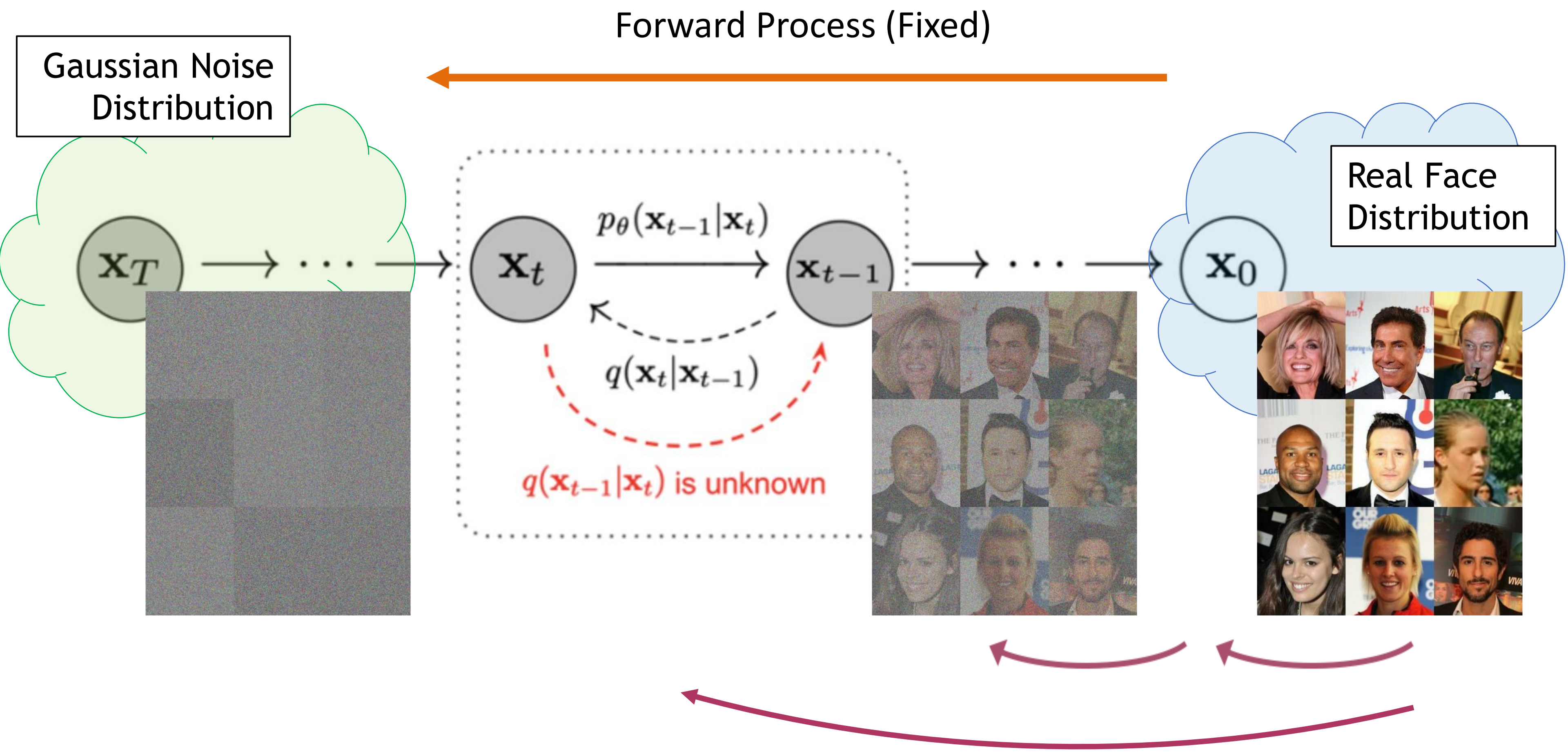
$$\mathcal{L}_{DIS} = \log\left(D\left(u_{\text{true}}\right)\right) + \log\left(1 - D\left(u_{\text{pred}}\right)\right).$$

DATA DRIVEN NO-EQUATIONS

[3] Deepak Pathak, Philipp Krahenbuhl, Jeff Donahue, Trevor Darrell, and Alexei A Efros. Context encoders: Feature learning by inpainting. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 2536–2544, 2016.

Li, T., Buzzicotti, M., Biferale, L., Bonaccorso, F., Chen, S., & Wan, M. (2023). Multi-scale reconstruction of turbulent rotating flows with proper orthogonal decomposition and generative adversarial networks. *Journal of Fluid Mechanics*, *971*, A3.

Forward Diffusion Process

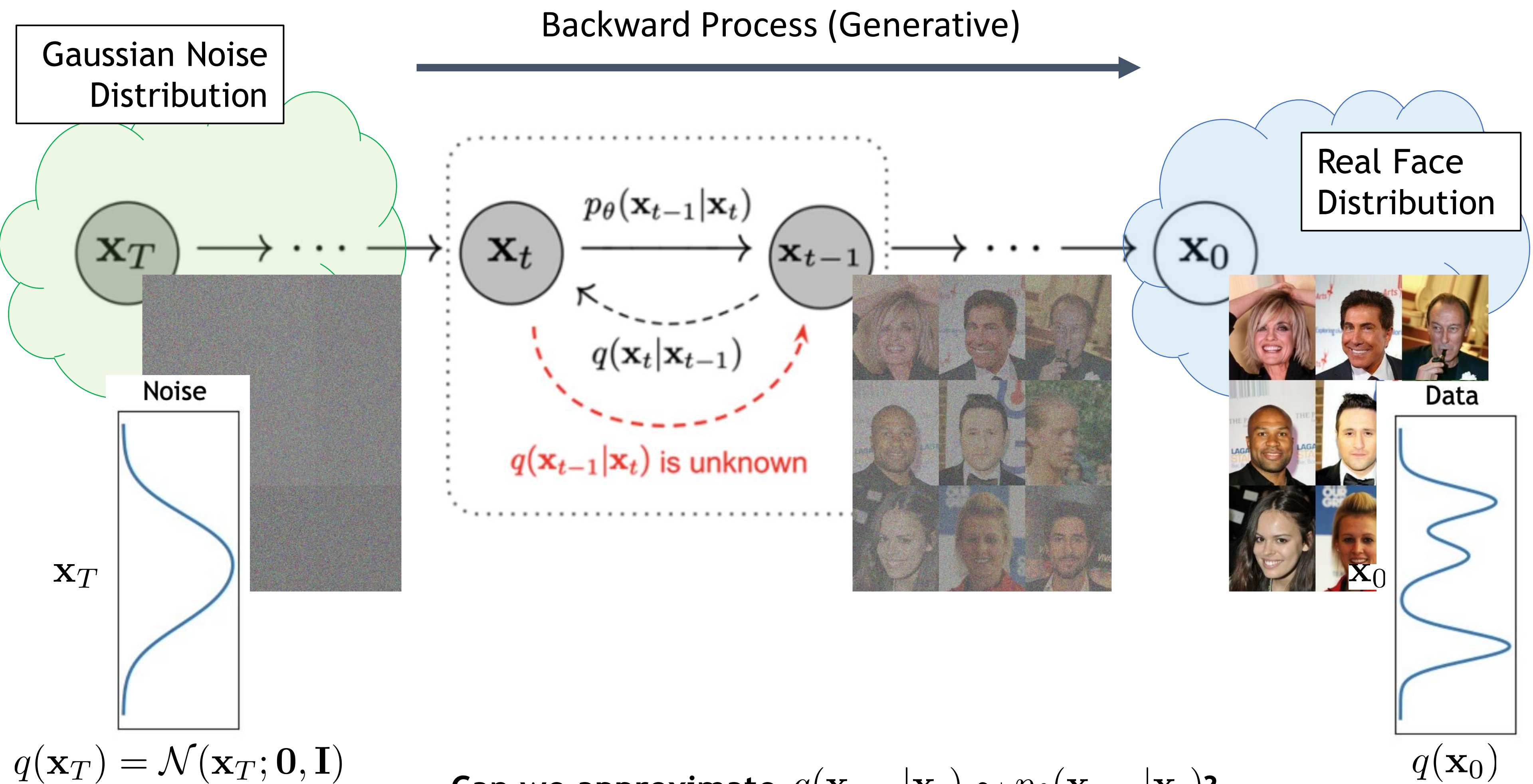


Define $\bar{\alpha}_t = \prod_{s=1}^{t}(1-\beta_s)$ ➡ $q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I}))$ (Diffusion Kernel)

For sampling: $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\,\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\,\epsilon$ where $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

β_t values schedule (i.e., the noise schedule) is designed such that $\bar{\alpha}_T \to 0$ and $q(\mathbf{x}_T|\mathbf{x}_0) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I}))$

Approx. Backward Diffusion Process

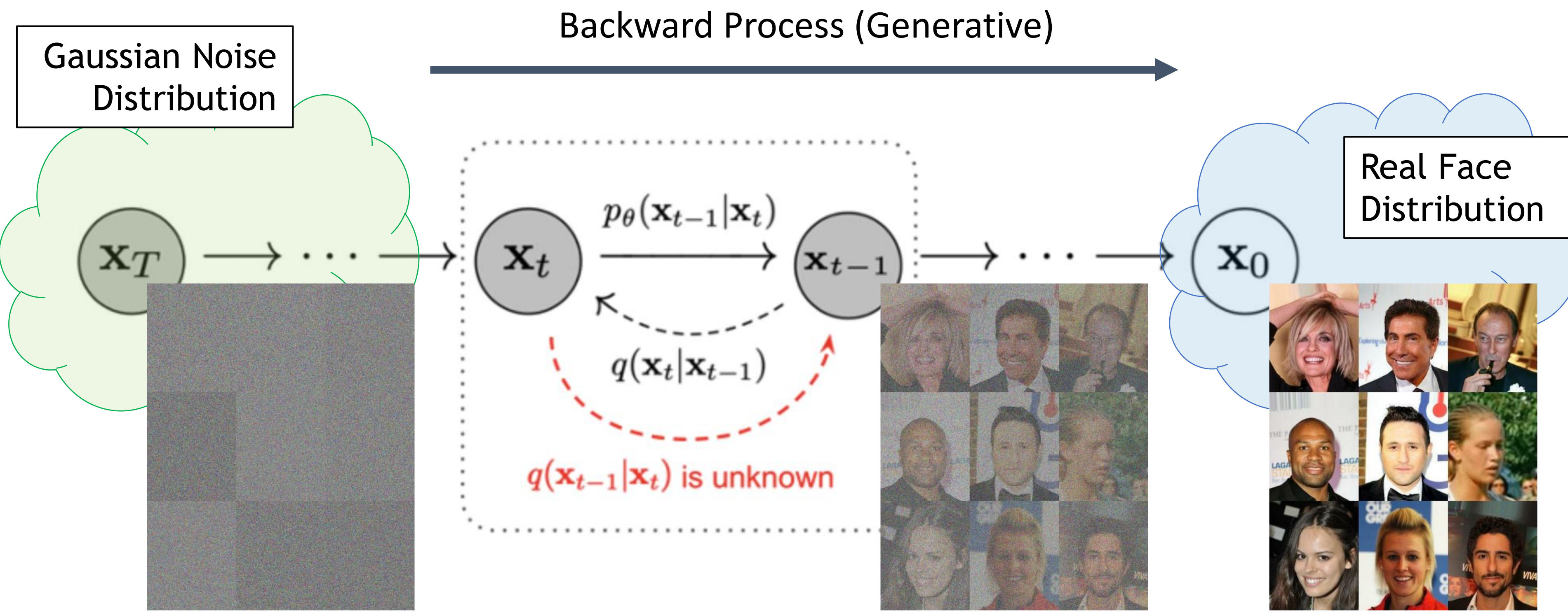


Can we approximate $q(\mathbf{x}_{t-1}|\mathbf{x}_t) \sim p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$**?**

$$\mathbf{x}_{t-1} \sim p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$$

Yes, we can use a Normal distribution if β_t is small in each forward diffusion step.

Recap [Main steps]



1) Backward step approximation → $q(\mathbf{x}_{t-1}|\mathbf{x}_t) \approx p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_\theta(\mathbf{x}_t, t), \sigma_t^2\mathbf{I})$

2) Optimization of the cross entropy → $\mathbb{E}_{q(\mathbf{x}_0)}[-\log p_\theta(\mathbf{x}_0)]$

3) Variational Upper Bound → $\mathbb{E}_{q(\mathbf{x}_0)q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right]$

4) Reparametrization of the Loss → $L_{t-1} \propto ||\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)||^2$