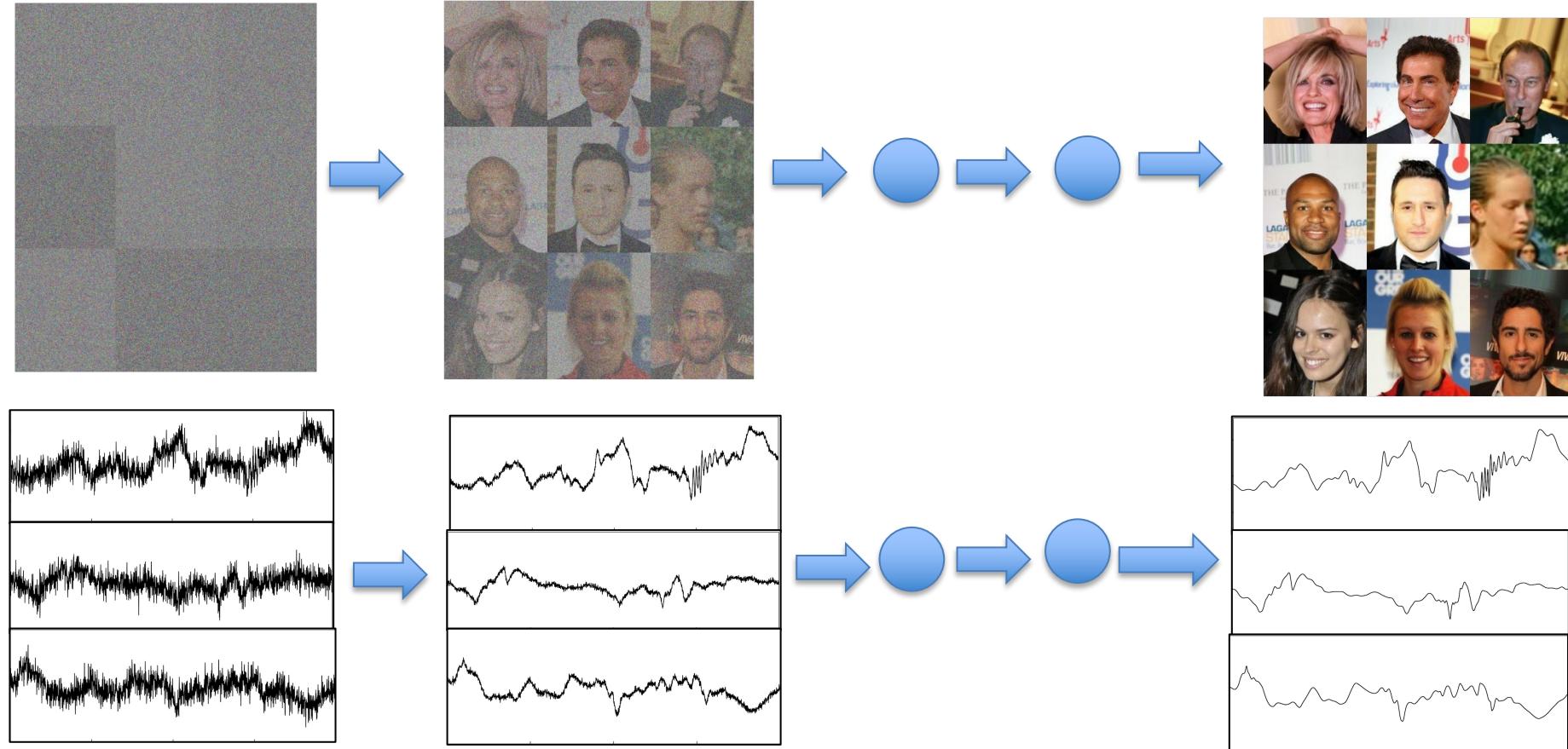




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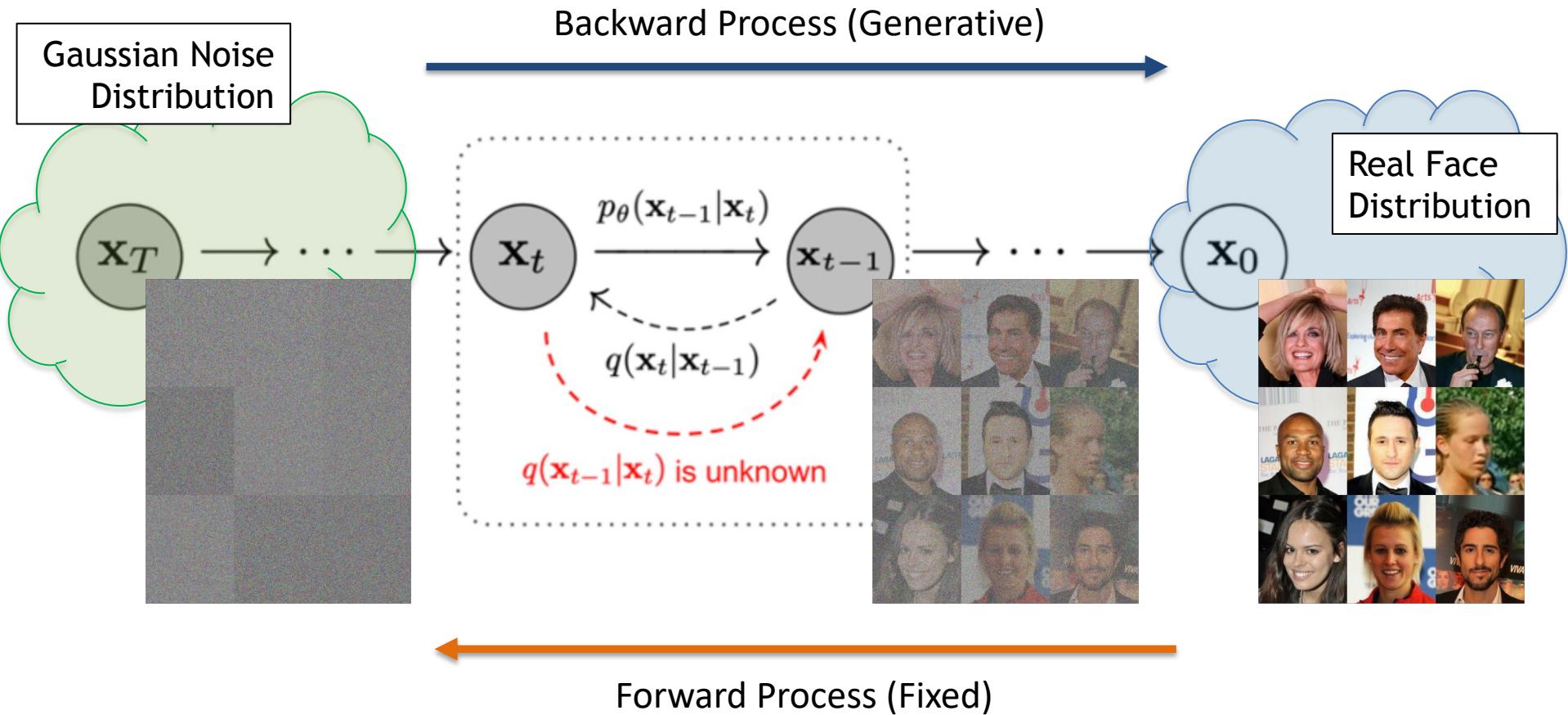
Complex Fluids and Complex Flows Group
Dept. Physics & INFN - University of Rome 'Tor Vergata'
michele.buzzicotti@roma2.infn.it
<https://mbuzzico.github.io/>



Synthetic Lagrangian Turbulence by Generative Diffusion Models

CREDITS: T. LI, L. BIFERALE, F. BONACCORSO, M. SCARPOLINI

Denoising Diffusion Models



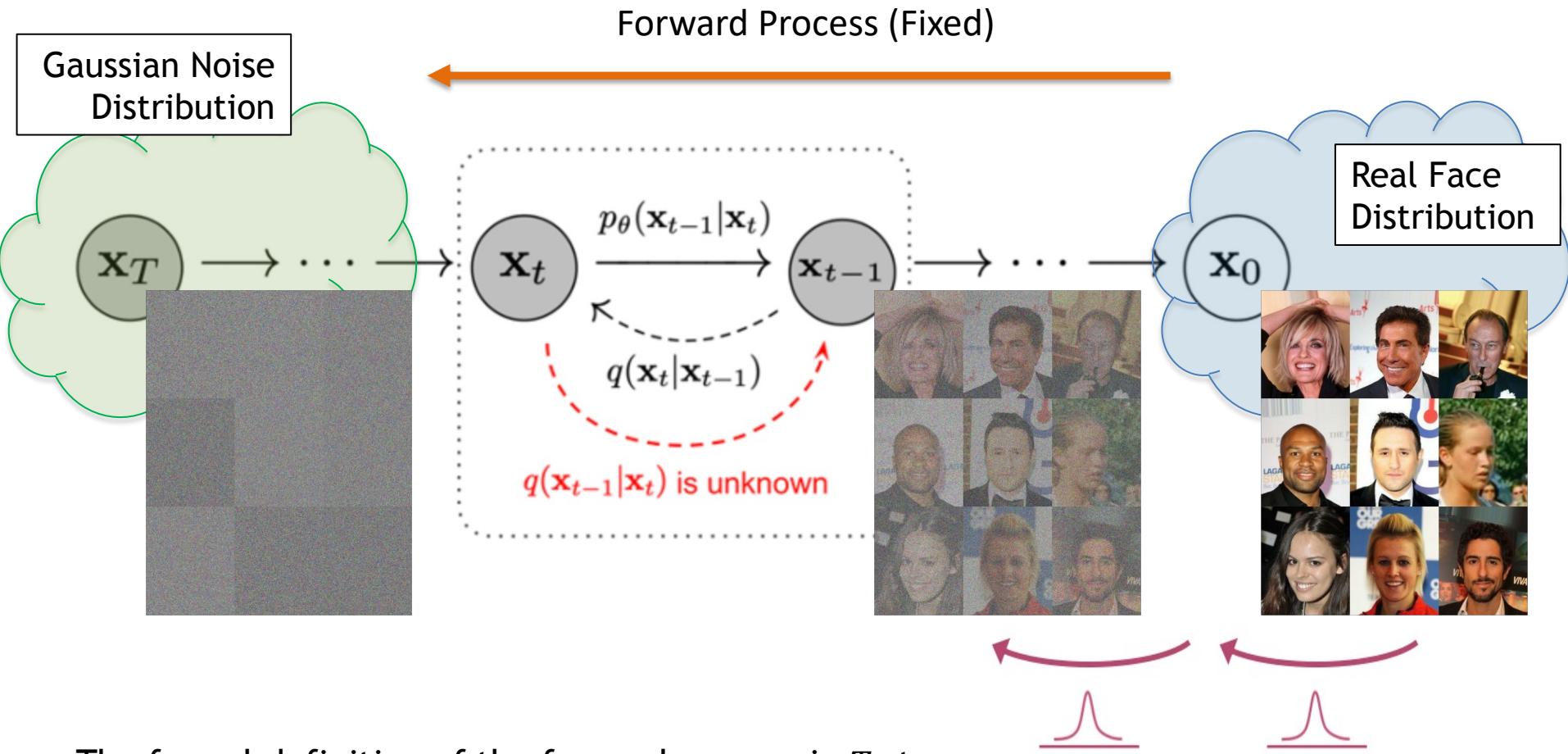
Learning to generate by denoising

[Sohl-Dickstein et al., Deep Unsupervised Learning using Nonequilibrium Thermodynamics, ICML 2015](#)

[Ho et al., Denoising Diffusion Probabilistic Models, NeurIPS 2020](#)

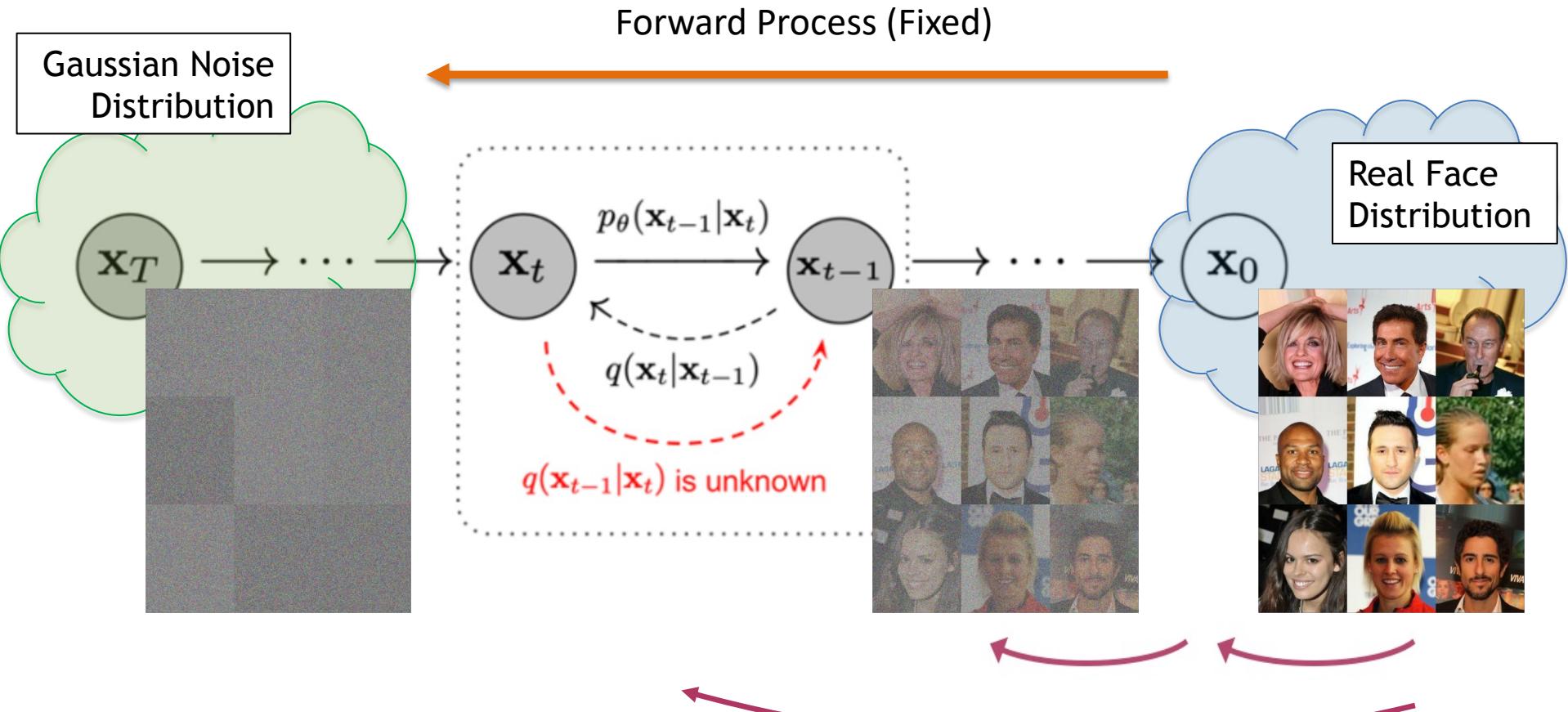
[Song et al., Score-Based Generative Modeling through Stochastic Differential Equations, ICLR 2021](#)

Forward Diffusion Process



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

Forward Diffusion Process

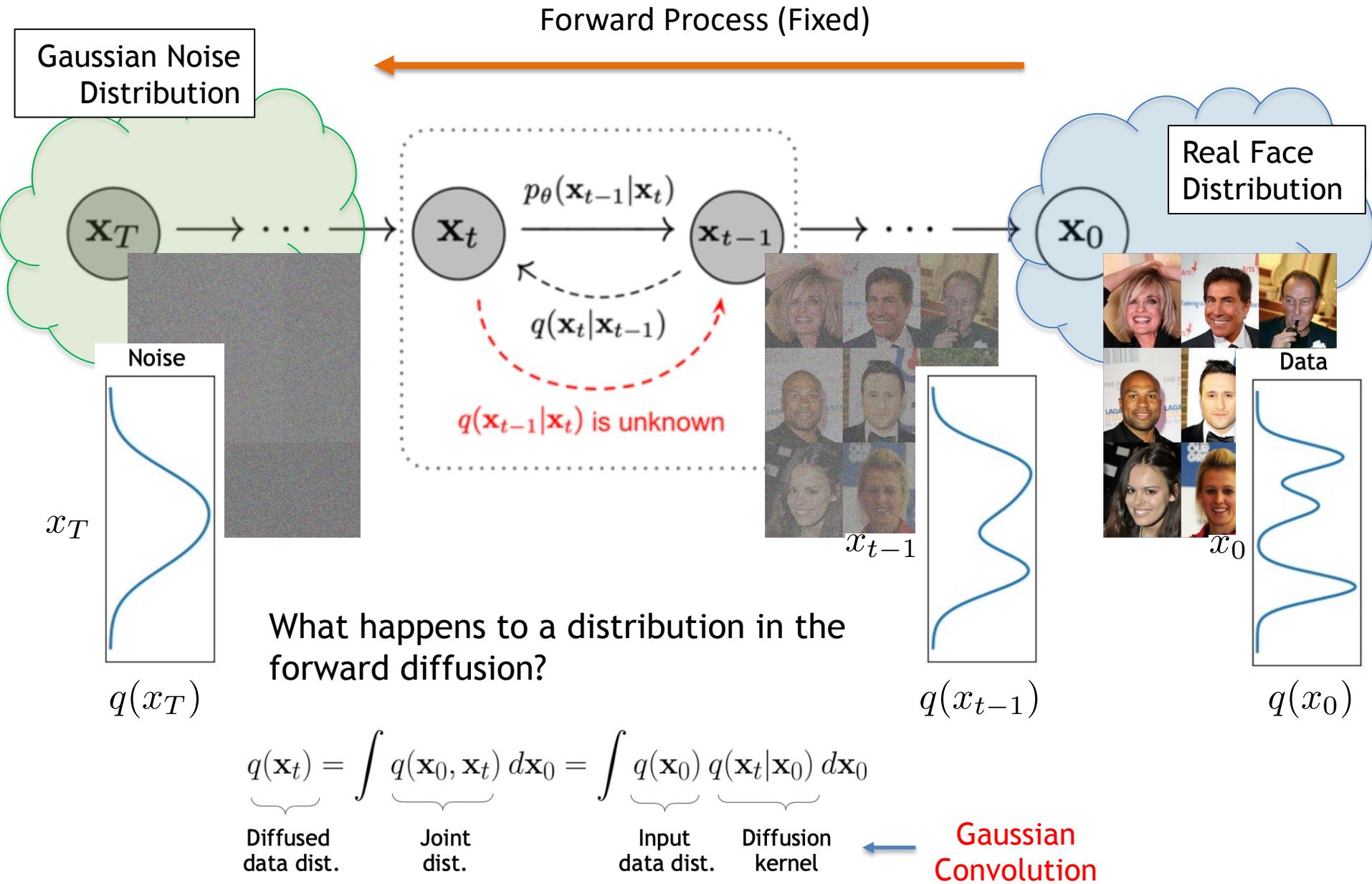


Define $\bar{\alpha}_t = \prod_{s=1}^t (1 - \beta_s)$ ➡ $q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I})$ (Diffusion Kernel)

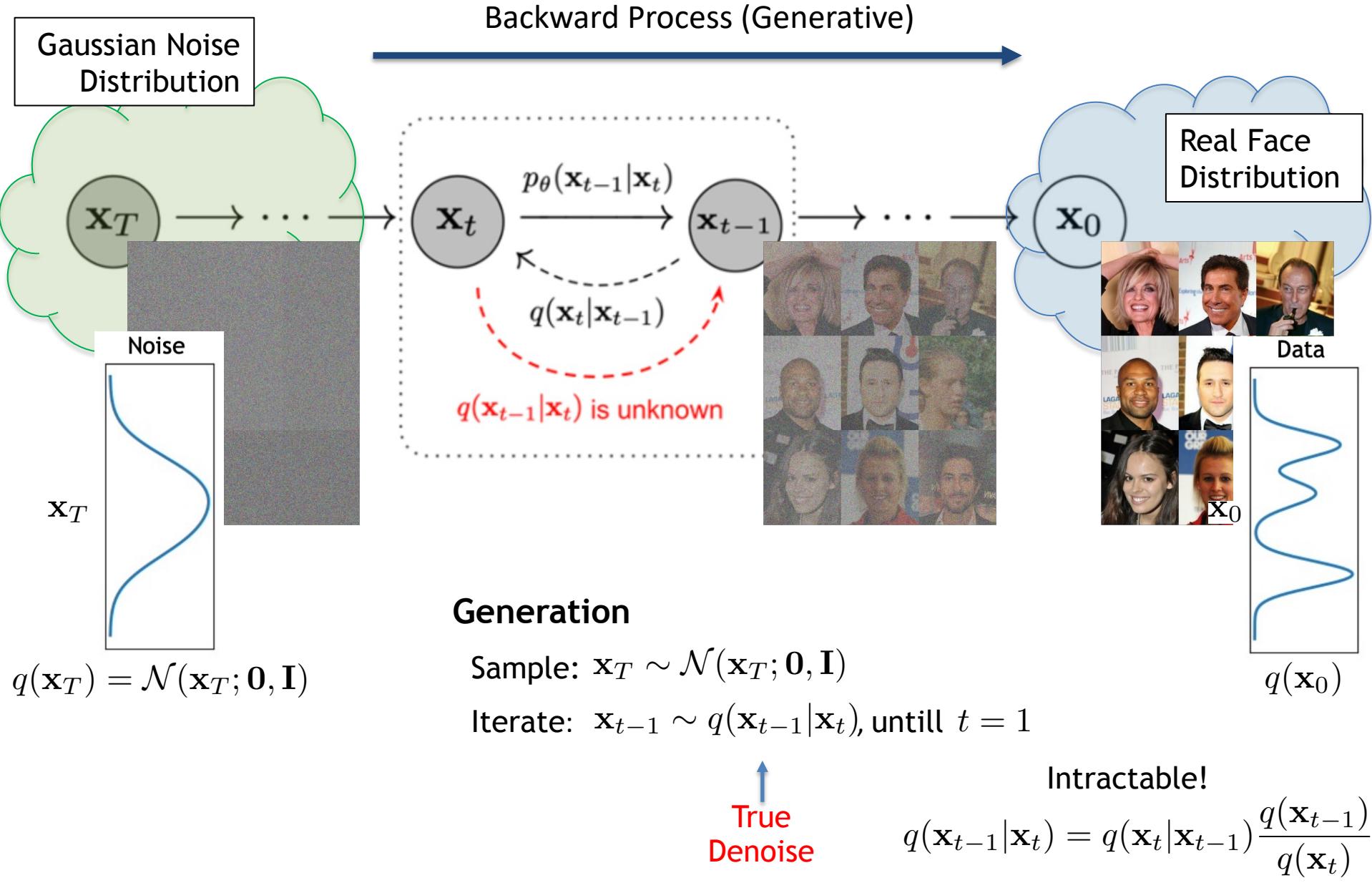
For sampling: $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{(1 - \bar{\alpha}_t)} \epsilon$ where $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

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

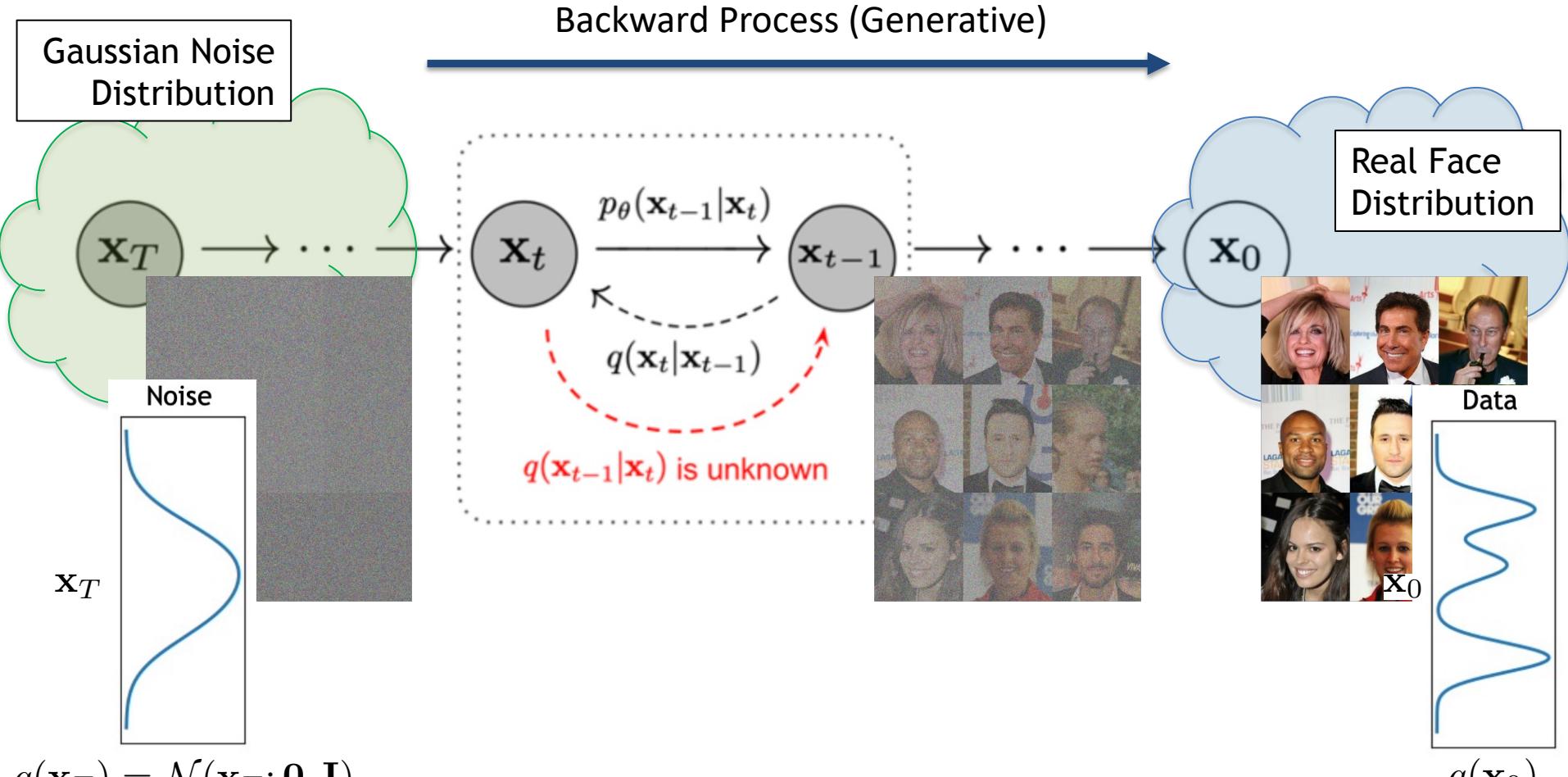
Forward Diffusion Process



Backward Diffusion Process



Approx. Backward Diffusion Process

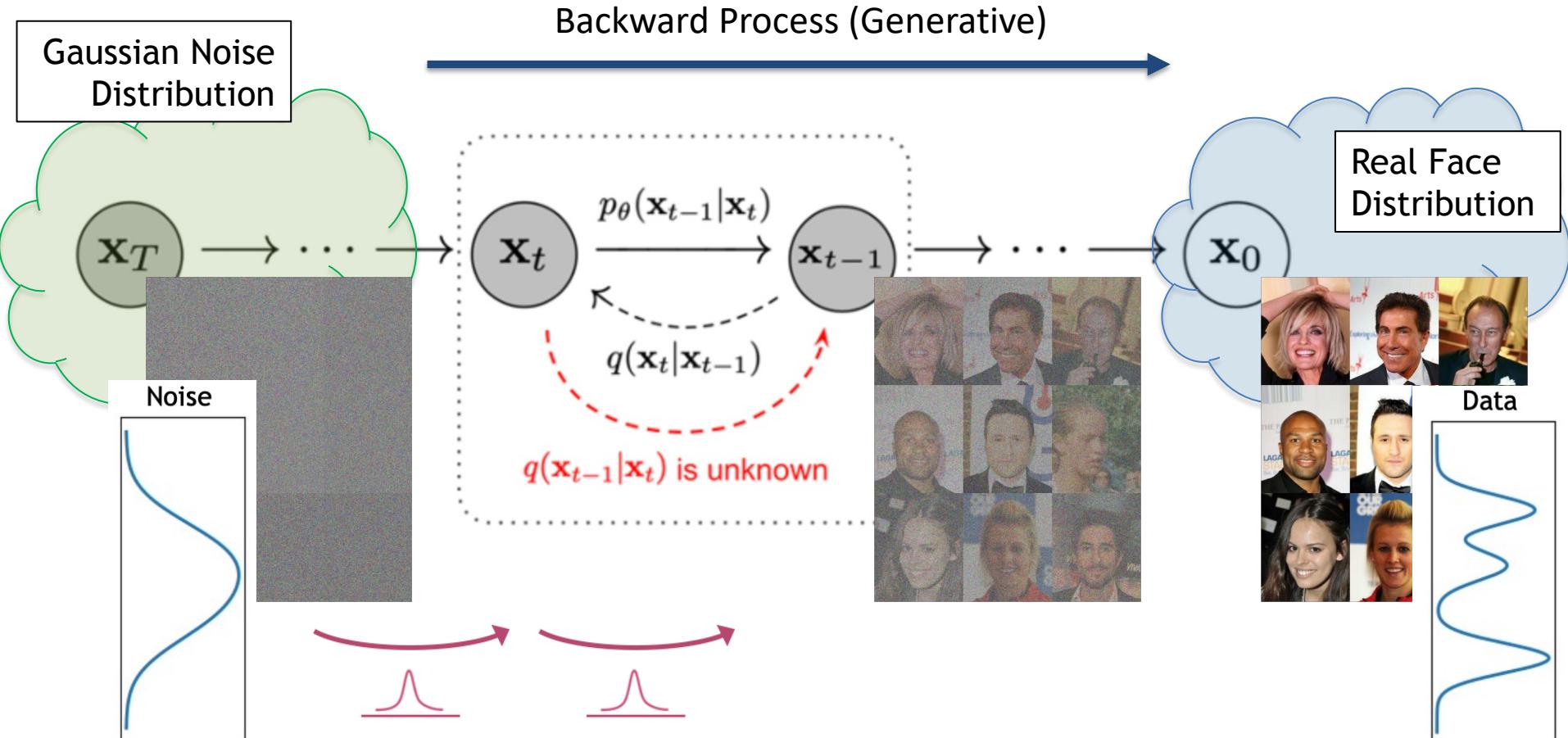


Can we approximate $q(\mathbf{x}_{t-1}|\mathbf{x}_t) \sim p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$?

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

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

Approx. Backward Diffusion Process



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

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \underbrace{\mu_\theta(\mathbf{x}_t, t)}, \sigma_t^2 \mathbf{I})$$

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

Trainable network (U-net, Denoising Autoencoder)

Learning the Backward Diffusion Process

Variational upper bound

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

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

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

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:

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

Learning the Backward Diffusion Process

Variational upper bound

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

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

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

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:

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

$$D_{KL}(p(x)||q(x)) = \int_{-\infty}^{+\infty} p(x) \log \left(\frac{p(x)}{q(x)} \right) dx \quad \text{KULLBACK-LEIBLER Divergence}$$

Learning the Backward Diffusion Process

Variational upper bound

$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ is the tractable posterior distribution:

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0) \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)}.$$

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \propto \exp\left(-\frac{(\mathbf{x}_t - \sqrt{\alpha_t}\mathbf{x}_{t-1})^2}{2\beta_t}\right) \cdot \exp\left(-\frac{(\mathbf{x}_{t-1} - \sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0)^2}{2(1-\bar{\alpha}_{t-1})}\right) \cdot \exp\left(\frac{(\mathbf{x}_t - \sqrt{\bar{\alpha}_t}\mathbf{x}_0)^2}{2(1-\bar{\alpha}_t)}\right)$$

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\tilde{\mu}(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_n \mathbf{I})$$

$$\text{where } \tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) := \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t} \mathbf{x}_0 + \frac{\sqrt{1-\beta_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t} \mathbf{x}_t \text{ and } \tilde{\beta}_t := \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t} \beta_t$$

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

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

$$D_{KL}(p(x)||q(x)) = \int_{-\infty}^{+\infty} p(x) \log \left(\frac{p(x)}{q(x)} \right) dx \quad \text{KULLBACK-LEIBLER Divergence}$$

Learning the Backward Diffusion Process

Variational upper bound

We need to evaluate the KL-Divergence between two Gaussians!

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \tilde{\mu}(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}) \quad p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_\theta(\mathbf{x}_t, t), \sigma_t^2 \mathbf{I})$$

We end up with the following Loss function:

$$L_{t-1} = D_{\text{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) || p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)) = \mathbb{E}_q \left[\frac{1}{2\sigma_t^2} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_\theta(\mathbf{x}_t, t)\|^2 \right]$$

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

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

$$D_{KL}(p(x)||q(x)) = \int_{-\infty}^{+\infty} p(x) \log \left(\frac{p(x)}{q(x)} \right) dx \quad \text{KULLBACK-LEIBLER Divergence}$$

Learning the Backward Diffusion Process

Variational upper bound

$$L_{t-1} = D_{\text{KL}}(q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) || p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)) = \mathbb{E}_q \left[\frac{1}{2\sigma_t^2} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_\theta(\mathbf{x}_t, t)\|^2 \right]$$

Recalling the properties of the forward process:

$$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) := \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 + \frac{\sqrt{1-\beta_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t \quad \mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)} \epsilon$$

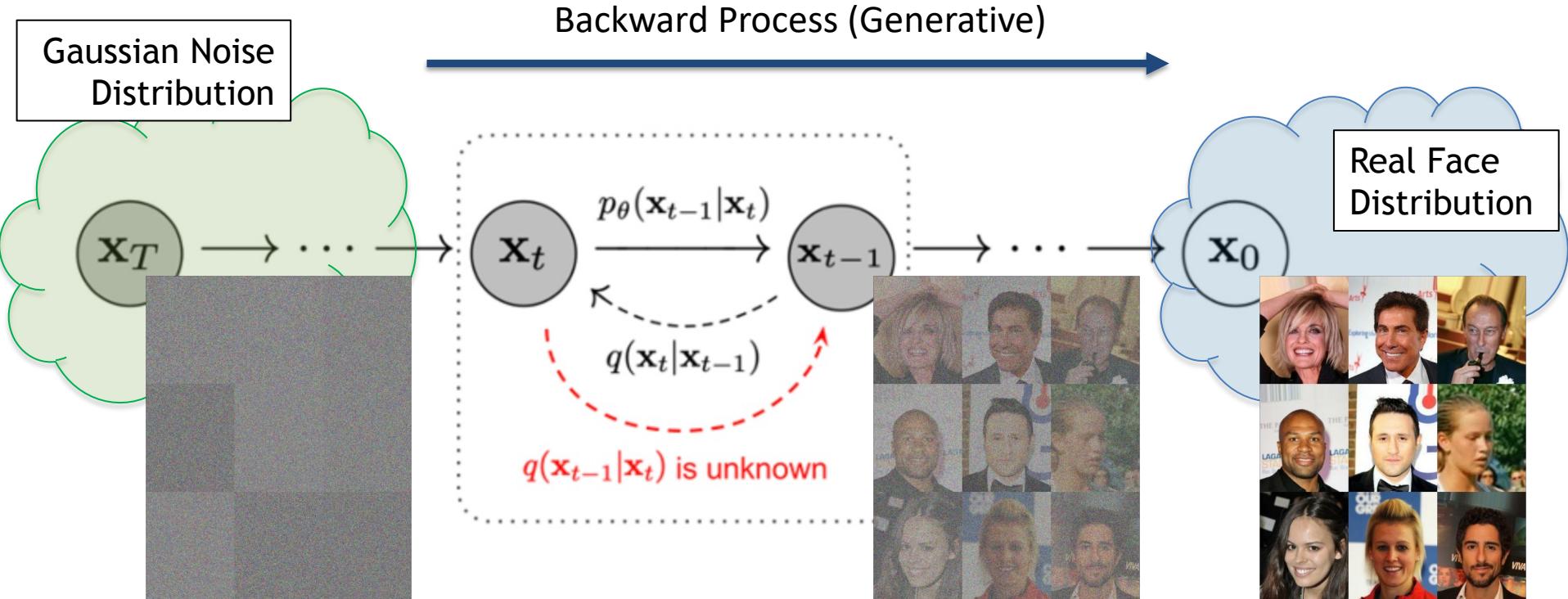
Ho et al. NeurIPS 2020 observed that:

$$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{1}{\sqrt{1-\beta_t}} \left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}} \epsilon \right) \quad \mu_\theta(\mathbf{x}_t, t) = \frac{1}{\sqrt{1-\beta_t}} \left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}} \epsilon_\theta(\mathbf{x}_t, t) \right)$$

They propose to **reparametrize the denoising model** using a *noise-prediction* network:

$$L_{t-1} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \left[\frac{\beta_t^2}{2\sigma_t^2(1-\beta_t)(1-\bar{\alpha}_t)} \|\epsilon - \underbrace{\epsilon_\theta(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t} \epsilon, t)}_{\mathbf{x}_t}\|^2 \right]$$

Recap [Main steps]



- 1) Backward step approximation $\rightarrow q(\mathbf{x}_{t-1}|\mathbf{x}_t) \approx p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_\theta(\mathbf{x}_t, t), \sigma_t^2 \mathbf{I})$
- 2) Optimization of the cross entropy $\rightarrow \mathbb{E}_{q(\mathbf{x}_0)}[-\log p_\theta(\mathbf{x}_0)]$
- 3) Variational Upper Bound $\rightarrow \mathbb{E}_{q(\mathbf{x}_0)q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \right]$
- 4) Reparametrization of the Loss $\rightarrow L_{t-1} \propto \|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)\|^2$

In Action

(Model Training and Sample Generation)

Algorithm 1 Training

```
1: repeat
2:    $\mathbf{x}_0 \sim q(\mathbf{x}_0)$ 
3:    $t \sim \text{Uniform}(\{1, \dots, T\})$ 
4:    $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
5:   Take gradient descent step on
      
$$\nabla_{\theta} \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}, t)\|^2$$

6: until converged
```

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{(1 - \bar{\alpha}_t)} \boldsymbol{\epsilon}$$

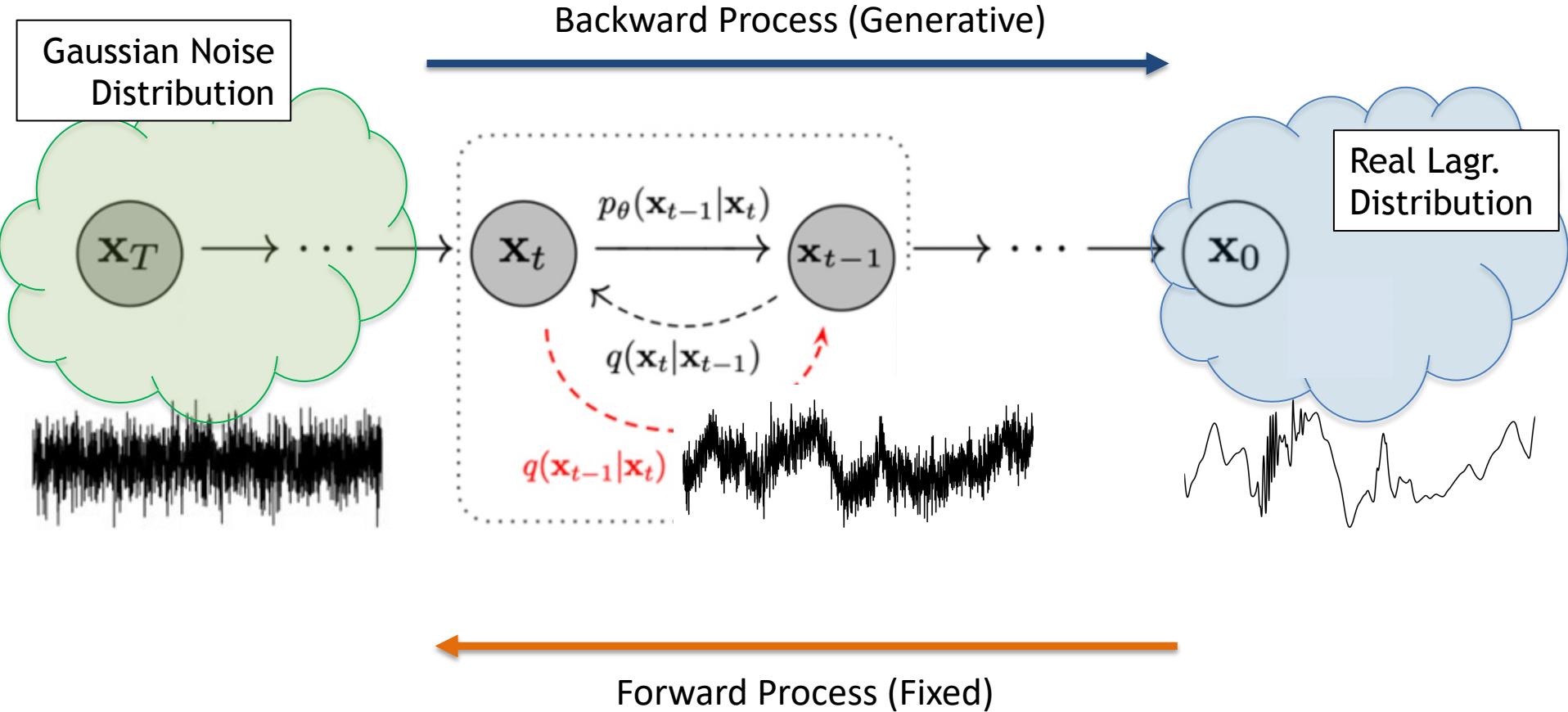
Algorithm 2 Sampling

```
1:  $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
2: for  $t = T, \dots, 1$  do
3:    $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
4:    $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left( \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$ 
5: end for
6: return  $\mathbf{x}_0$ 
```

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

$$\mu_{\theta}(\mathbf{x}_t, t) = \frac{1}{\sqrt{1 - \beta_t}} \left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1 - \bar{\alpha}_t}} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t) \right)$$

Diffusion Models for Lagrangian Turbulence



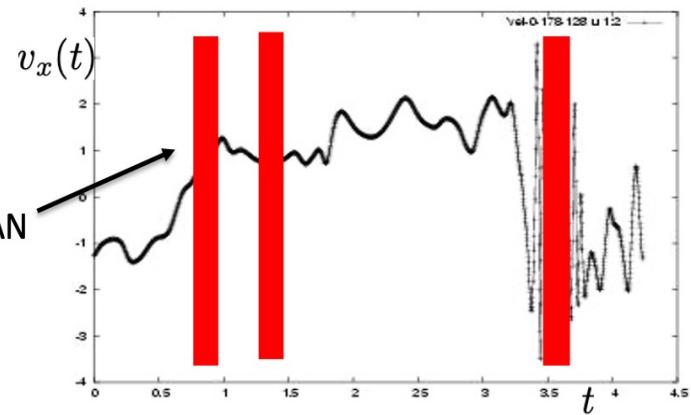
T. Li, L. Biferale, F. Bonaccorso, M. Scarpolini and M. Buzzicotti.
Synthetic Lagrangian Turbulence by Generative Diffusion Models.
arXiv:2307.08529 (2023) - Submitted to Nature Machine Intelligence

STOCHASTIC MODELS FOR LAGRANGIAN TURBULENCE: WHY?

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

DATA ASSIMILATION/INPAINTING FROM MISSING FIELD/EXPERIMENTAL OBSERVATION

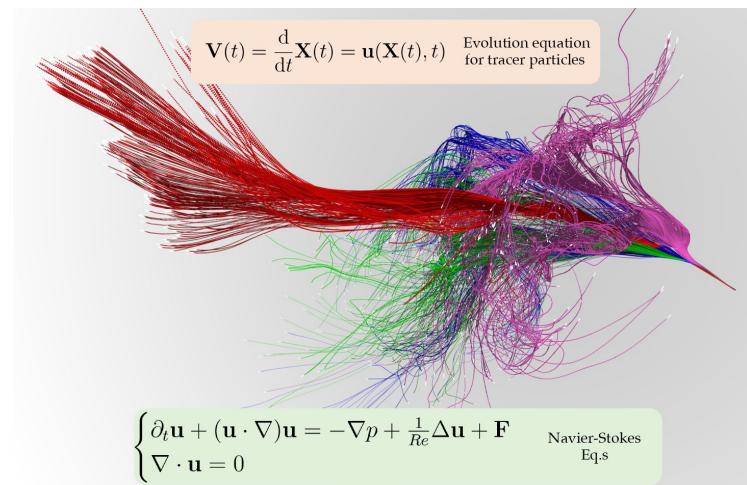
LAGRANGIAN



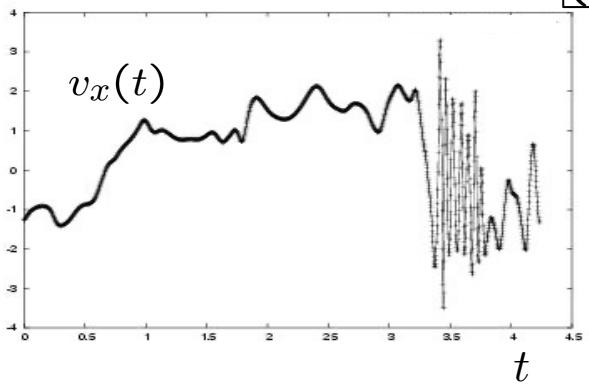
CLASSIFICATION/INFERRAL OF MISSING/INTERNAL PROPERTIES:

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

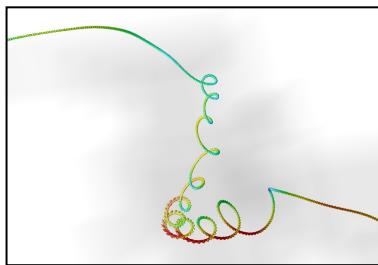
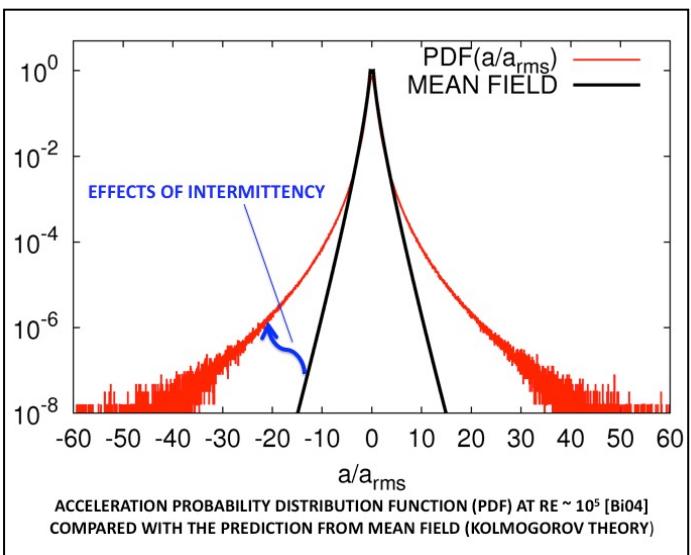
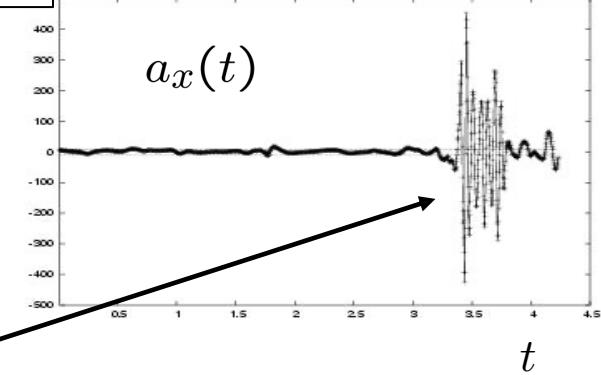
→



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



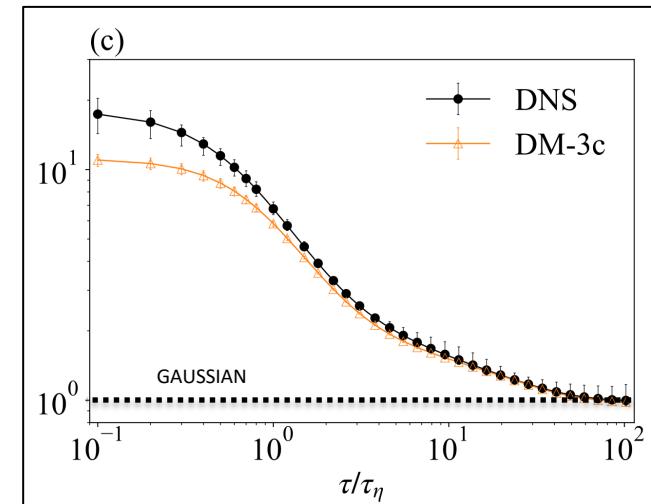
EXTREME EVENTS



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

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

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

~30 years of modeling experience

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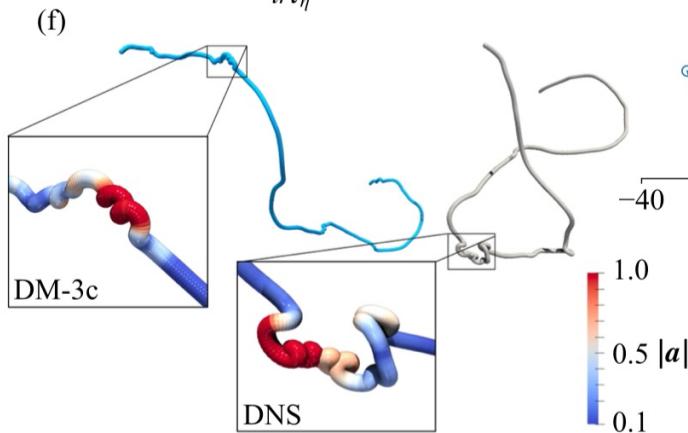
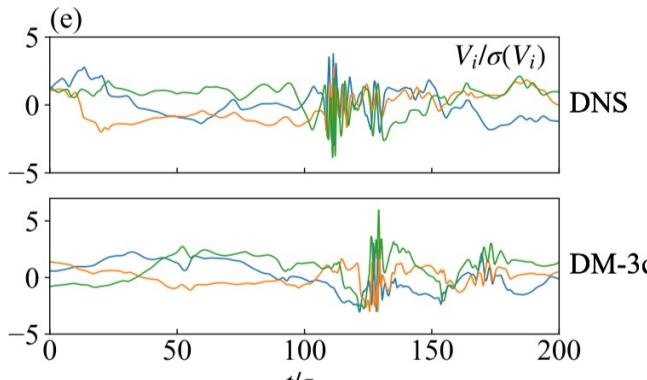
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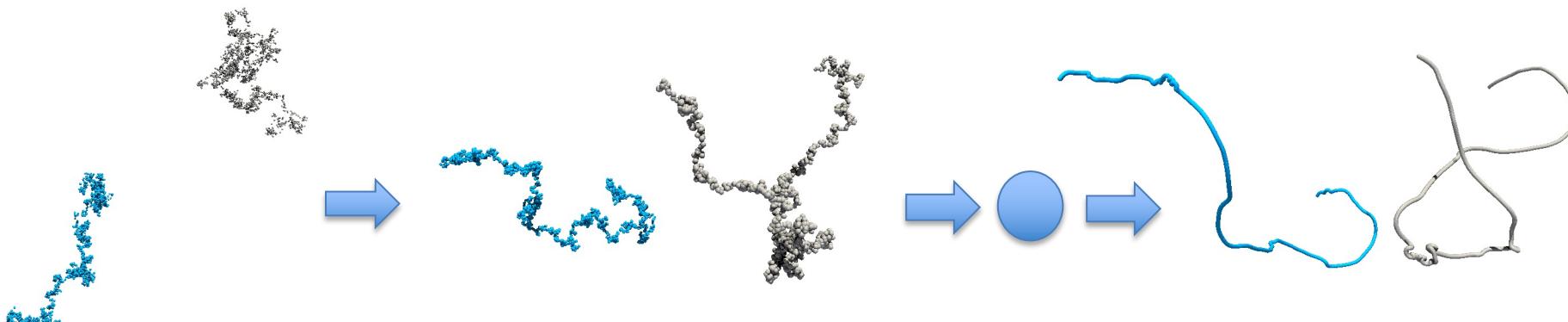
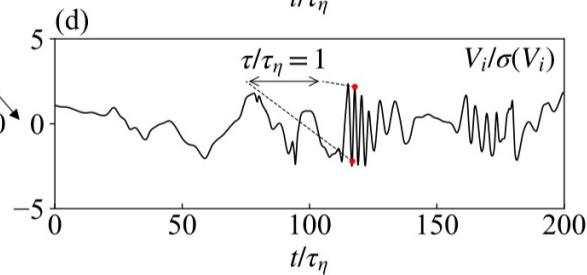
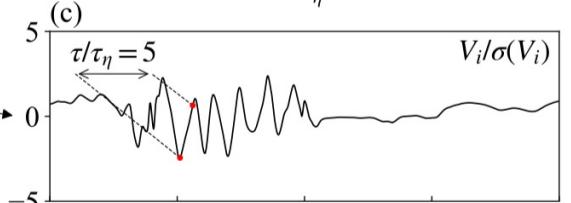
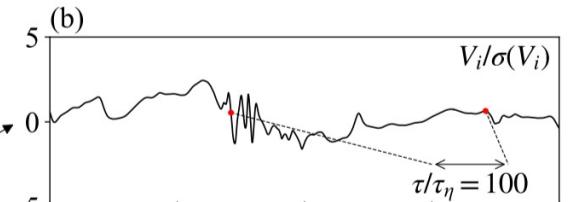
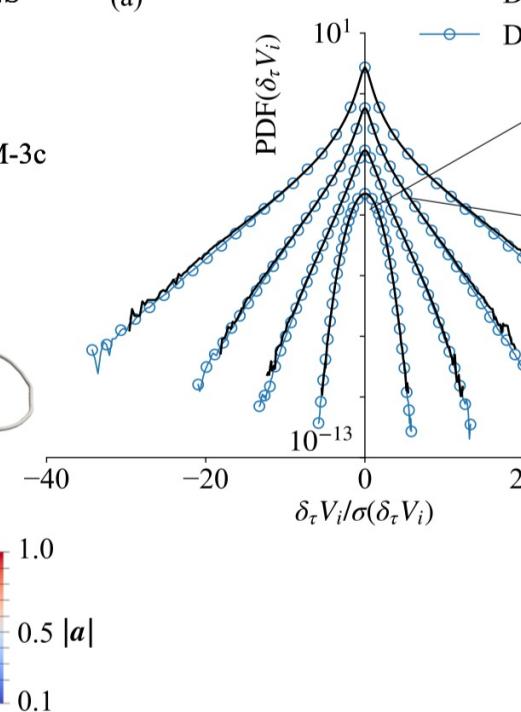
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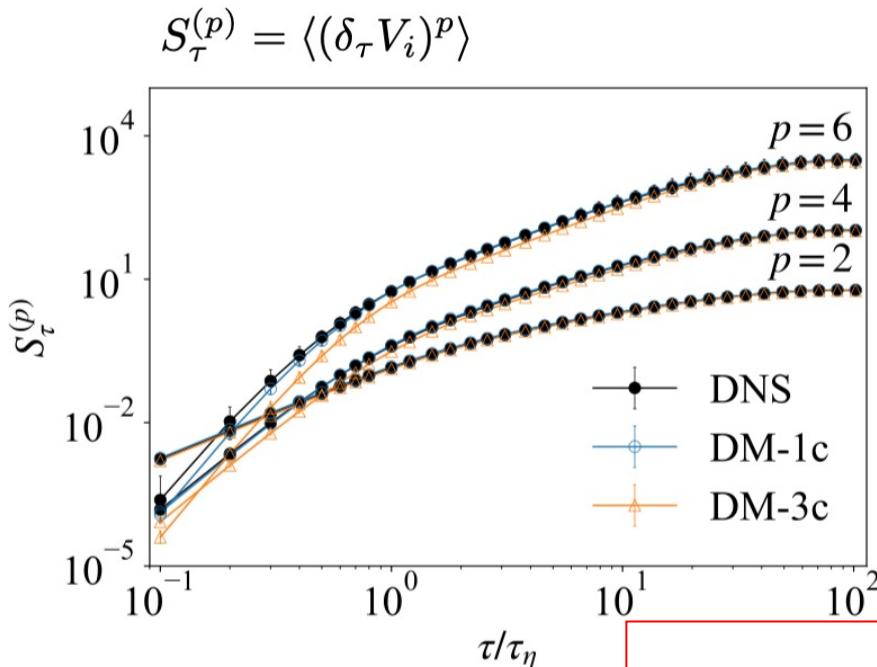
$$\delta_\tau V_i(t) = V_i(t + \tau) - V_i(t),$$



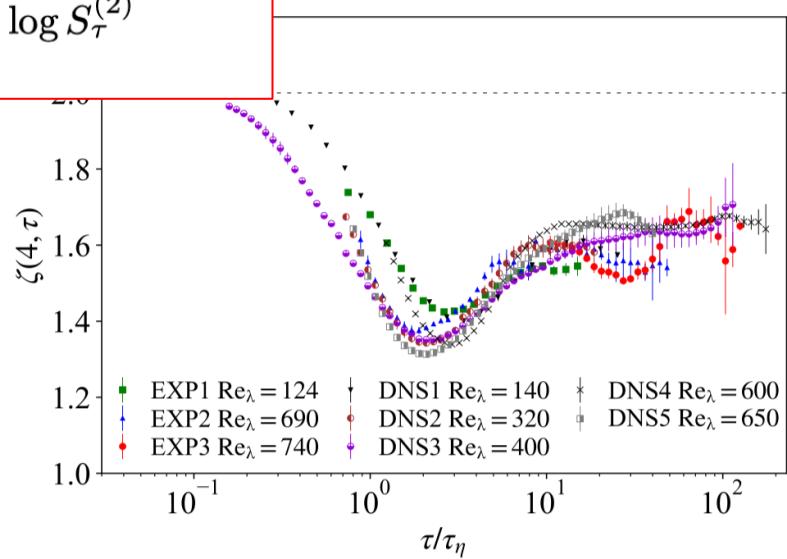
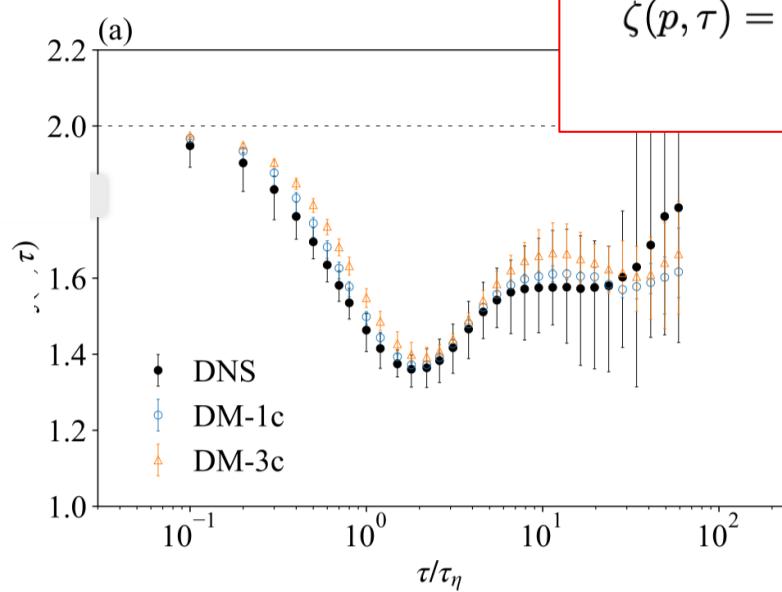
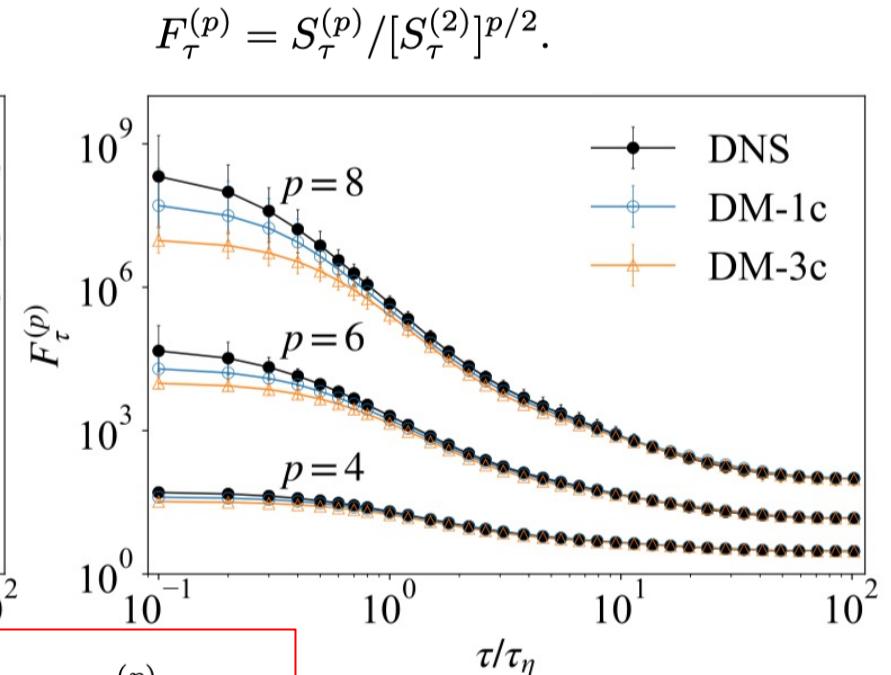
(a)



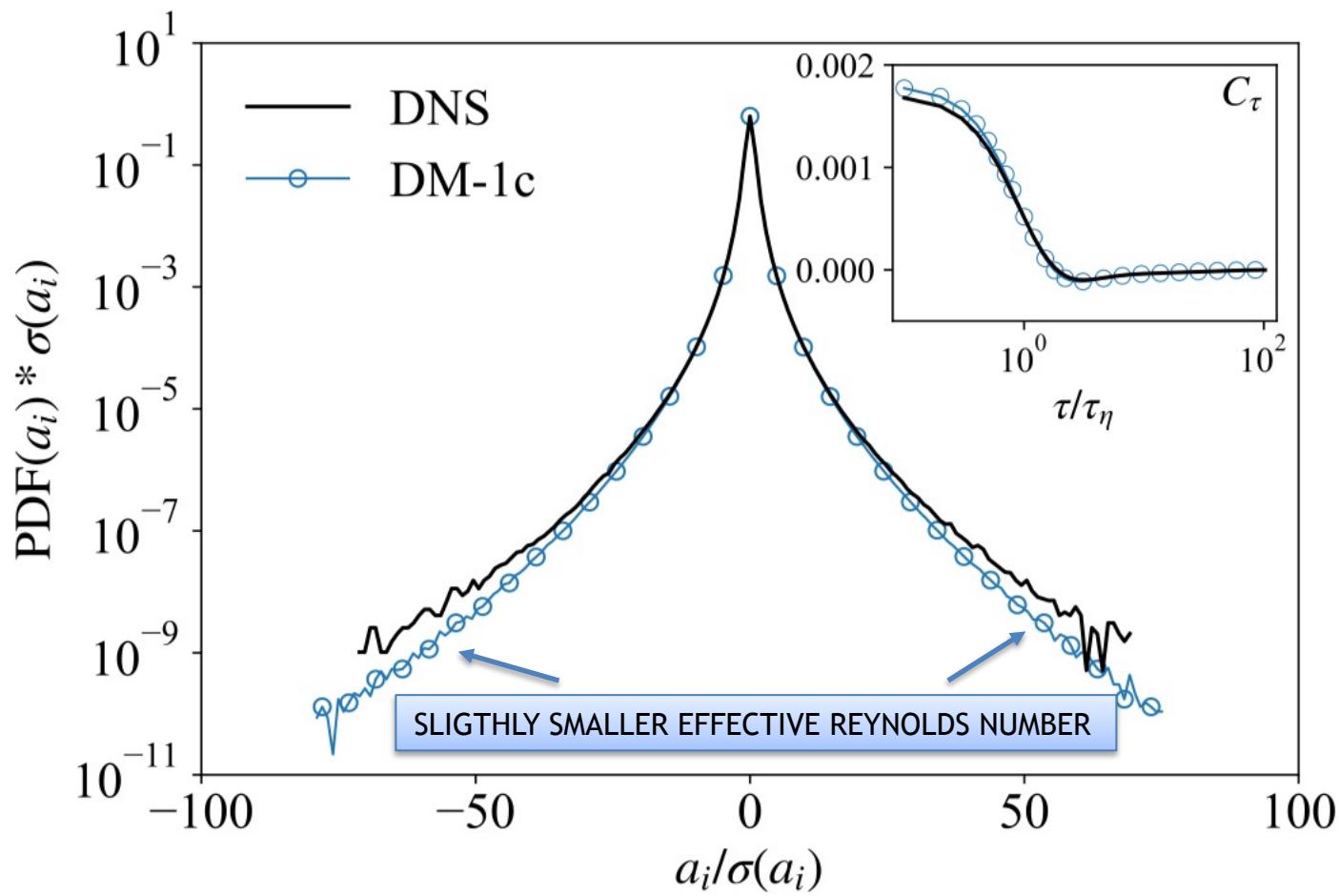
LAGRANGIAN STRUCTURE FUNCTIONS

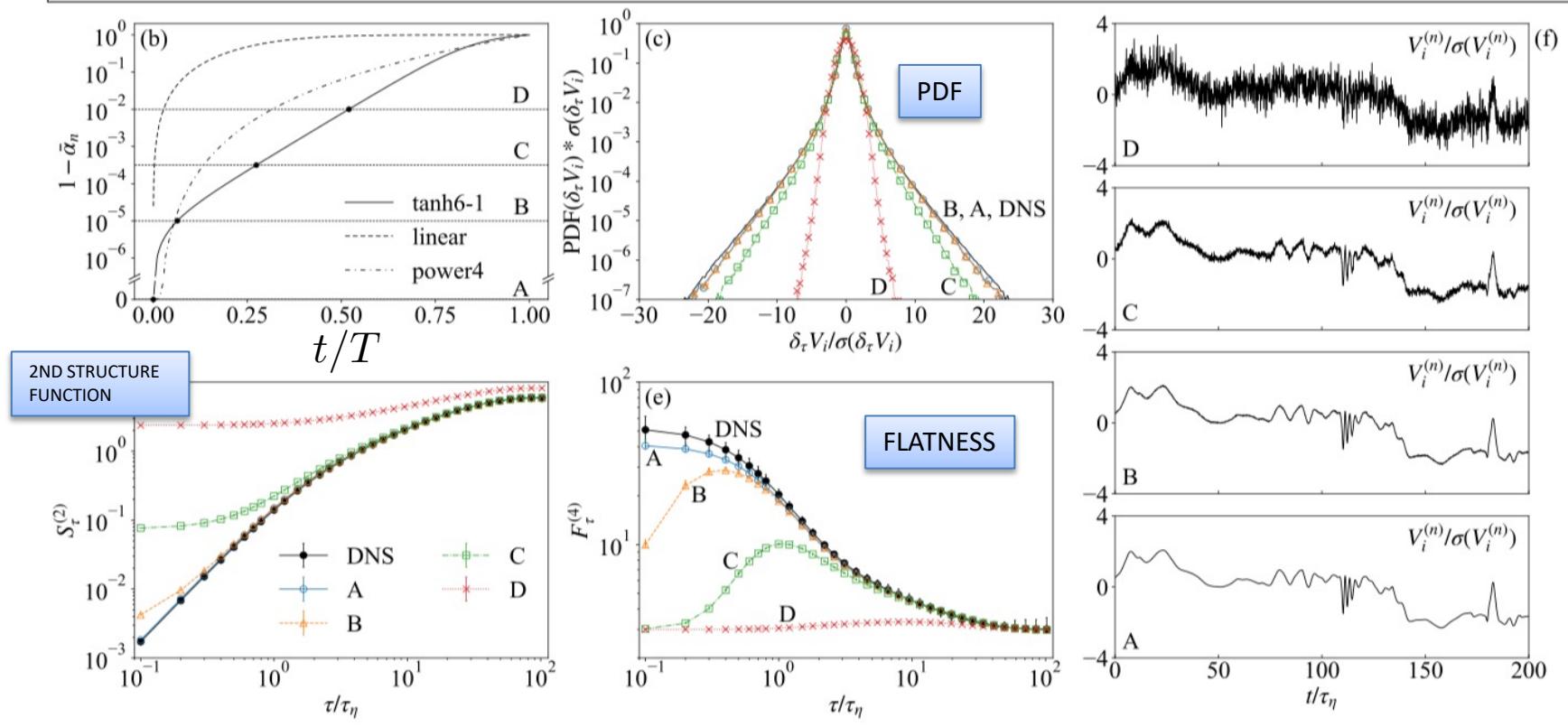
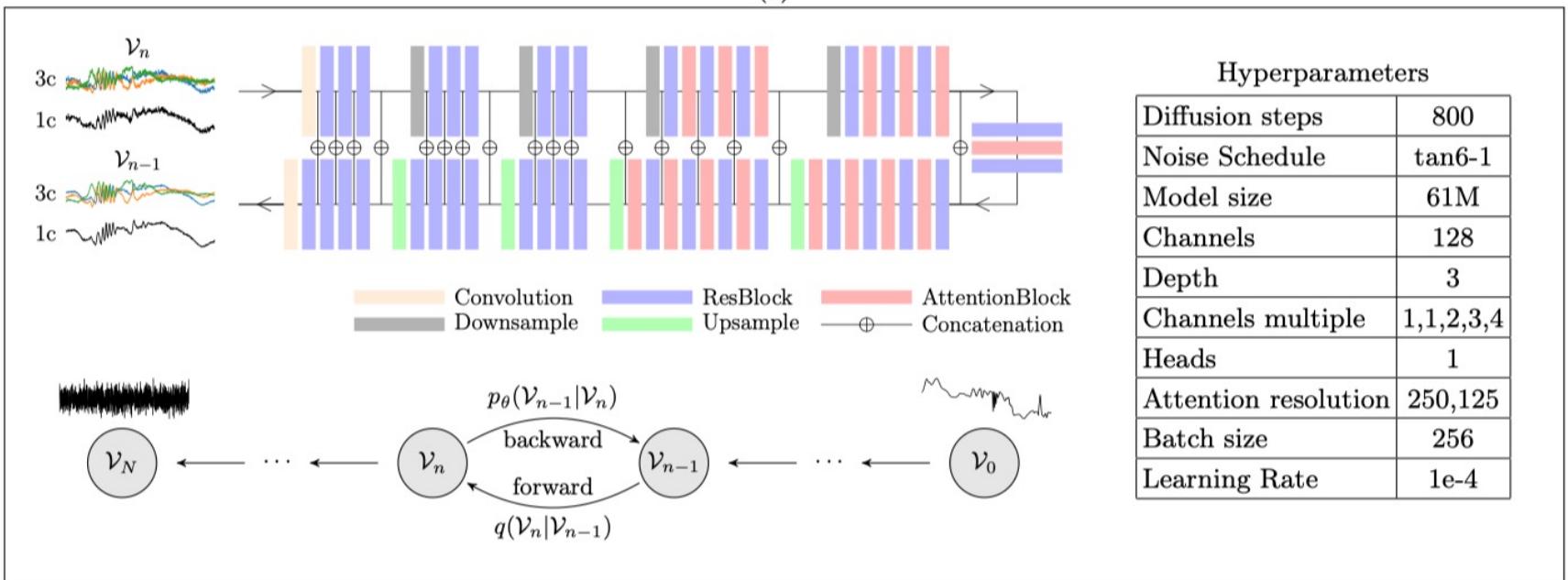


GENERALIZED FLATNESS



ACCELERATION PDF





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

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



Guide for users

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. Bonacorso
Center for Life Nano Sciences @La Sapienza
Istituto Italiano di Tecnologia and INFN
University of Rome Tor Vergata, Italy.
fabio.bonacorso@roma2.infn.it

M. Buzzicotti
Dept. Physics and INFN
University of Rome Tor Vergata, Italy.
michele.buzzicotti@roma2.infn.it

P. Clark Di Leon
Department of Mechanical Engineering,
Johns Hopkins University, Baltimore, USA.
pato@jhu.edu

Search for datasets

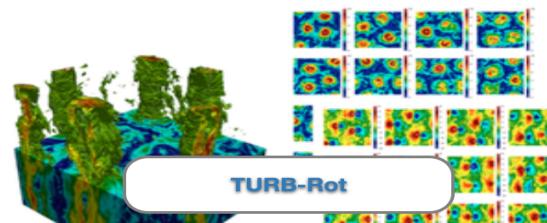


1

Datasets

TURB-Rot

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



2

Organizations

web_admin

web_admin group

1 member