

Easy Electrospinning

Towards Multimodal Generative Inverse Design of
Electrospun Nanofibres Using Experimental Parameters and
SEM-based Morphology Representations

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Project jointly proposed by: the BioFab and IFSB teams of UTC's BMBI laboratory.

- * BioFab: Biomatériaux et Fabrication de Tissus
- * IFSB : Interactions Fluides-Structures Biologiques
- * BMBI : BioMécanique et BioIngénierie UMR CNRS 7338
- * UTC : Université de Technologie de Compiègne

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1 Electrospinning and Electrospun Fibres

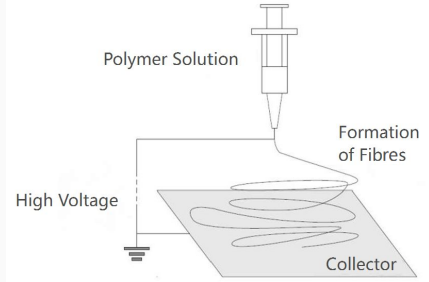


Fig. Standard electrospinning setup



Fig. Device used to generate the *EPs_Explore_1d8k* dataset: TL-PRO electrospinning machine from Shenzhen Tongli Micro-Nano Technology Co., Ltd. Device size: 1100 mm × 730 mm × 950 mm.

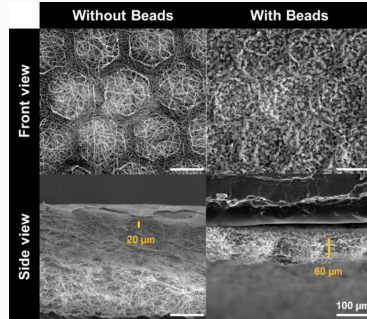


Fig. Example of research conducted at the UTC-BMBI laboratory on electrospun scaffolds for cell culture. Left: SEM images of honeycomb-structured scaffolds with and without bead-on-string fibres. Right: Epifluorescence images showing Live/Dead staining after 6 days of cell culture on different scaffolds.

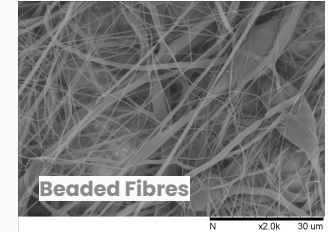
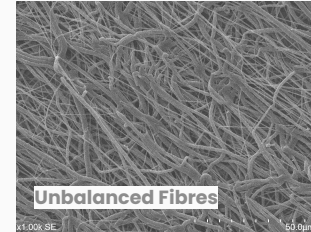
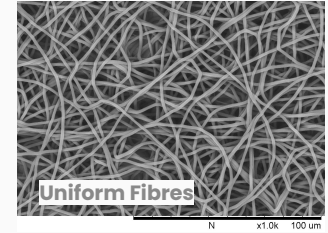
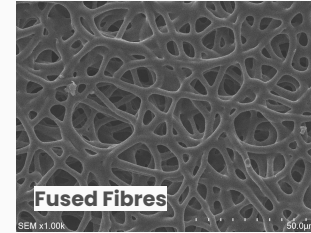
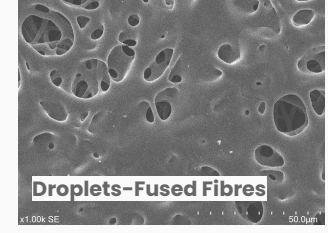
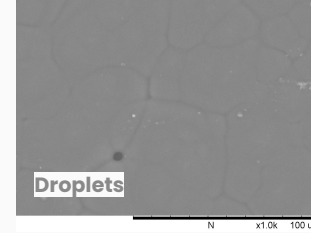
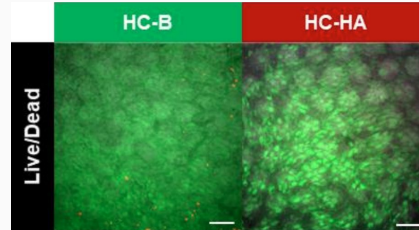


Fig. Representative fibre morphologies observed in electrospinning experiments. Data from the UTC-BMBI laboratory.

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2.1 Coupled Multiphysics Mechanisms in Electrospinning

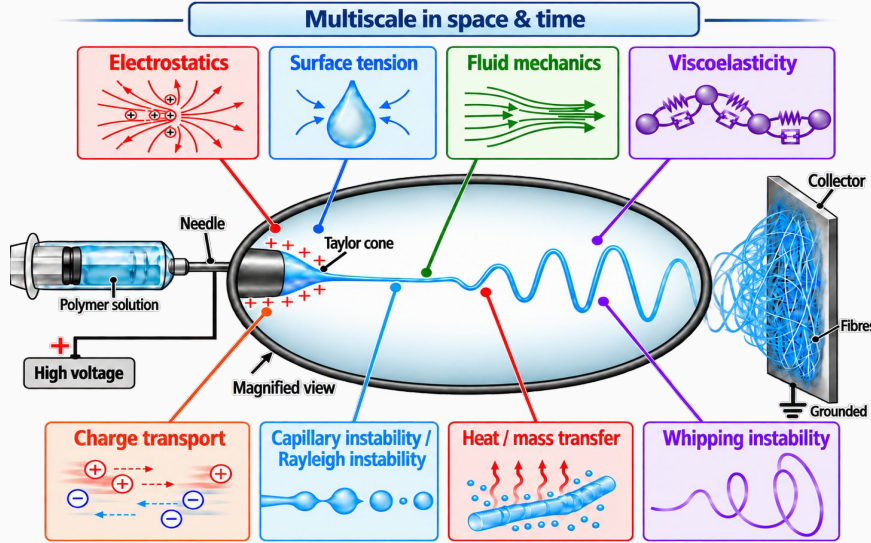


Fig. Coupled multiphysics mechanisms in electrospinning. Schematic generated with the assistance of DALL-E (OpenAI).

Tab. Examples of Key Dimensionless Groups in Electrospinning Jet Stability Analysis

Parameter	Dimensionless number	Definition
Re	Reynolds No.	$\frac{\rho v_0 R_0}{\eta}$
We	Weber No.	$\frac{\rho v_0^2 R_0}{\gamma}$
Pe	Electric Péclet No.	$\frac{2 \bar{\epsilon} v_0}{K R_0}$
Fr	Froude No.	$\frac{v_0^2}{g R_0}$
α	Field strength	$\frac{\bar{\epsilon} E_0^2}{\rho v_0^2}$
E_∞	Imposed potential diff.	$\frac{\Delta V / L}{E_0}$
β	Relative permittivity	$\frac{\epsilon}{\bar{\epsilon}} - 1$
χ	Jet aspect ratio	$\frac{L}{R_0}$
r_η	Polymer viscosity ratio	$\frac{\eta_p}{\eta_s + \eta_p}$
De	Deborah No.	$\frac{\lambda v_0}{R_0}$

- **Key challenge:** Coupling physical mechanisms across multiple spatial and temporal scales while accounting for realistic material properties and experimental conditions.

2.2 Coupled Mechanisms in Electrospinning: A Representative Example

PIB Boger fluid – Oldroyd-B Model

- Low conductivity
- Capillary-dominated instability
- Relatively simple viscoelastic response

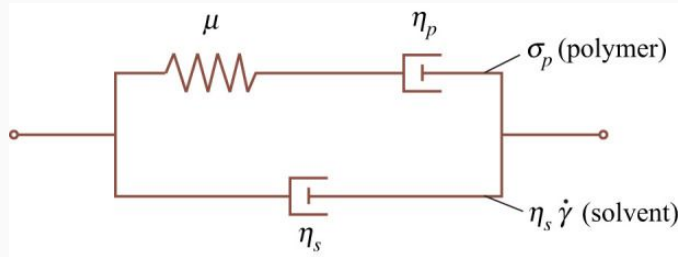


Fig. Qualitative representation of the Oldroyd-B fluid.

PEO solution – XPP Model

- High conductivity
- Electrically driven conducting mode
- Nonlinear extensional response under strong stretching

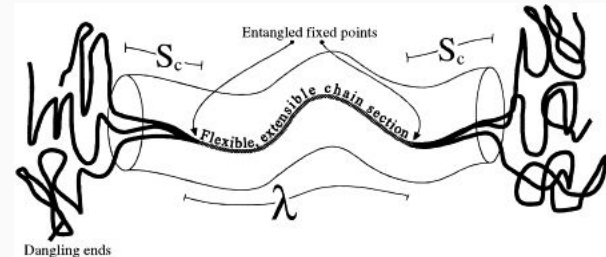


Fig. Three-armed pom-pom molecule

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3.1 Towards Generative Inverse-Design – Graphical Overview of the Project

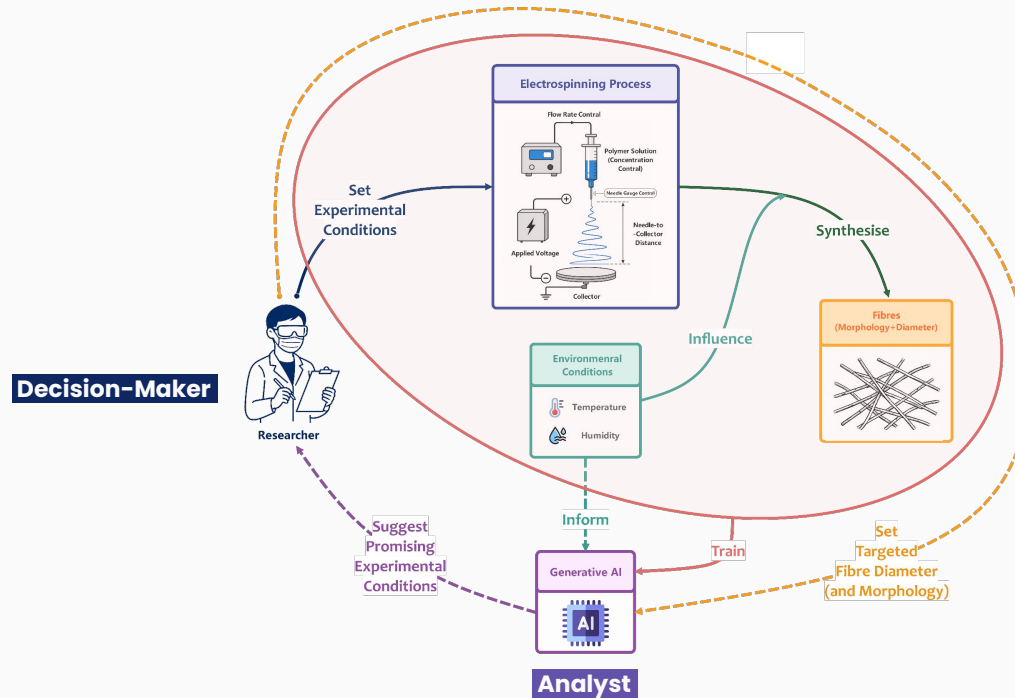
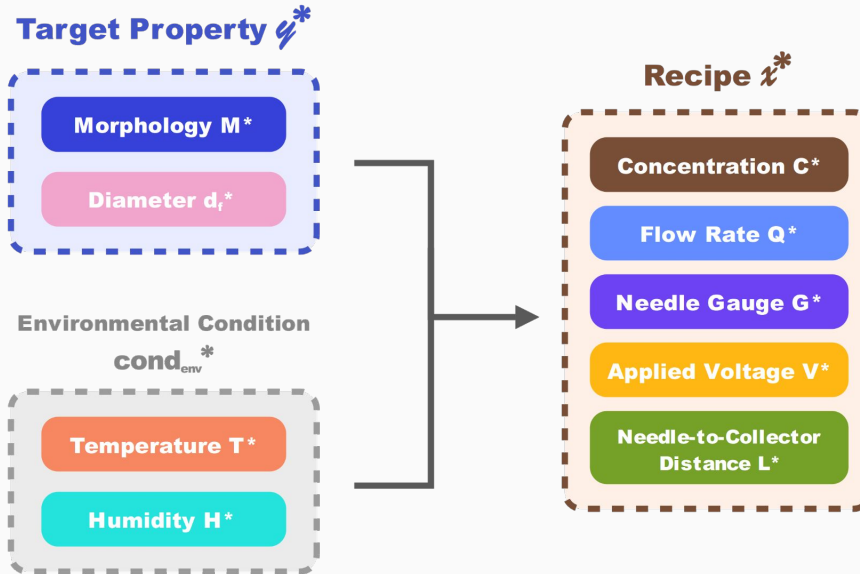


Fig. Schematic overview of the electrospinning process and the proposed generative inverse-design framework.

3.2 Problem Formulation

- **Objective:** model the process–structure relationship across the full range of electrospinning regimes



- $M \in \{\text{droplets, droplets-fused fibres, fused fibres, fibres}\}$

- Existing scaling law

$$d_f \propto \left[\frac{\eta_0 Q K^{0.2} L^2}{\Delta V^2} \right]^{1/2}$$

- d_f : Diameter
 - η_0 : Viscosity
 - Q : Flow Rate
 - K : Conductivity
 - L : Needle-to-collector distance
 - ΔV : Applied voltage
- Related to solute(s), solvent(s), and solution concentration
Not routinely measured or actively controlled

3.3 Idealised Illustration of the Output of a Conditional Generative AI Model

- Illustration of $P(C, Q, G, V, L | M, d_f, T, H)$ after projecting the 5D recipe space onto 2D using PCA :

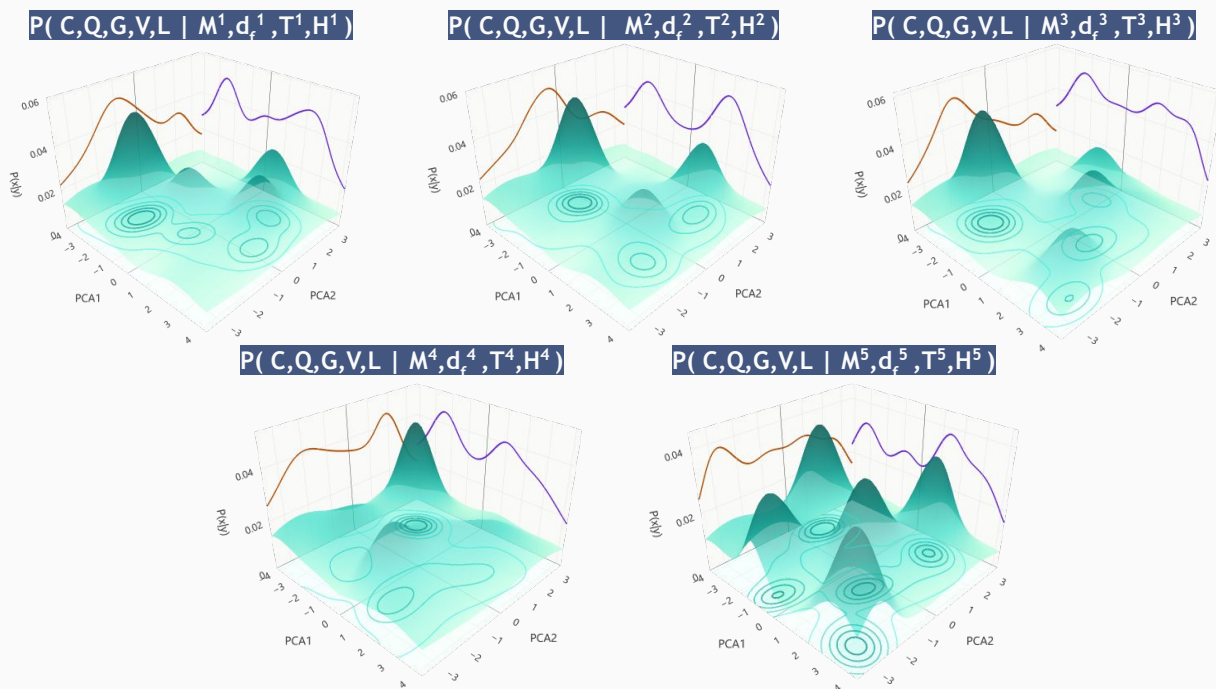


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4.1 Two Target Fibre Properties

Fibre Diameter

- Quantitative information from SEM images
- Manual measurements → diameter distribution
- Common descriptors:
 - Mean
 - Standard Deviation
 - Coefficient of Variation (Uniformity)
- Widely used in existing studies

Fibre Morphology

- Visual / structural information from SEM images
- Often represented by discrete labels
- Evolves continuously across regimes:
 - Droplets;
 - Fused fibres;
 - Fibres
 - ...
- **Often not explicitly included in modelling**

4.2 Quantify Diameter Uniformity using Diameter Statistics – Coefficient of Variation (CV)

$$CV = \frac{STD}{MEAN}, \quad CV \in (0, +\infty)$$

CV captures only **diameter variability**,
not the full structural characteristics.

⇒ **Need: A complementary metric** for
overall fibre morphology

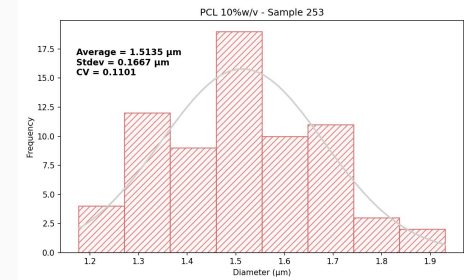
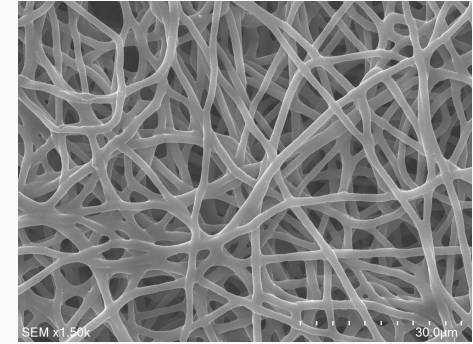
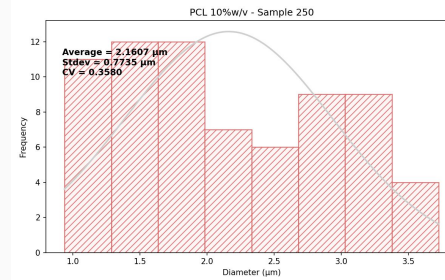
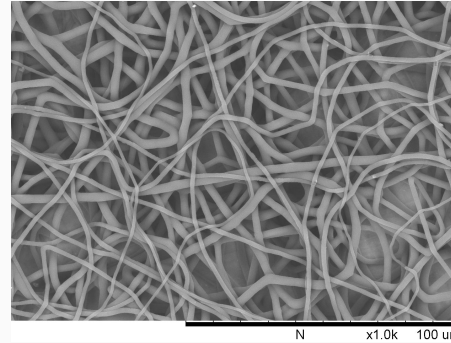
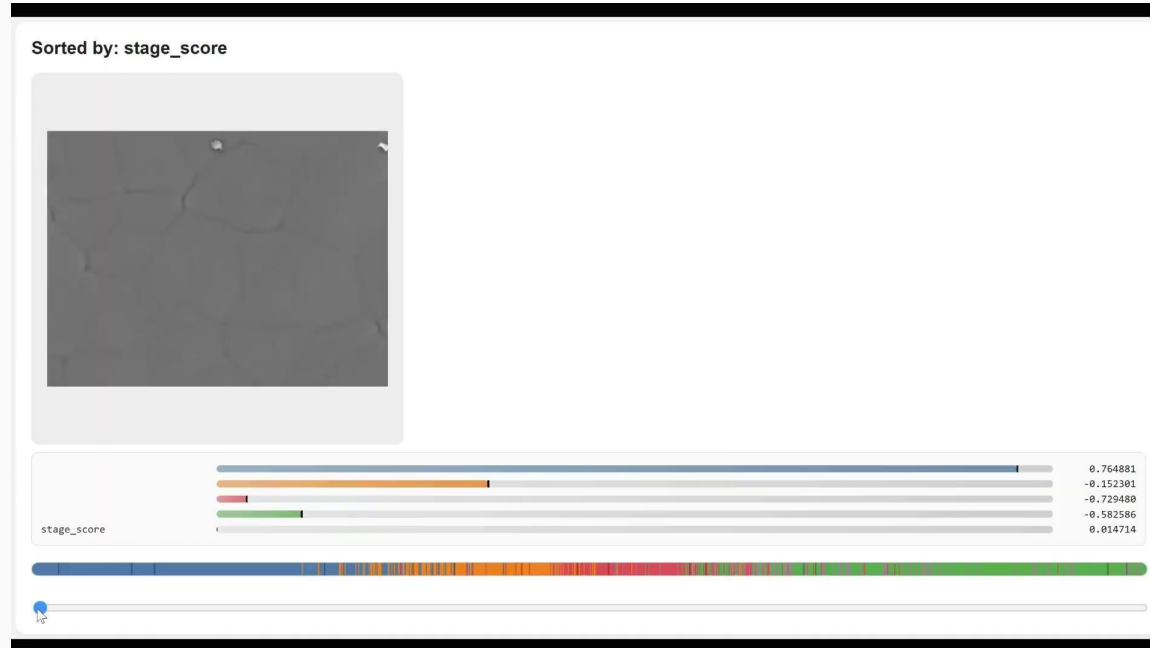


Fig. SEM images and fibre diameter distributions of samples 10%-250 (left) and 10%-253 (right).

4.3 SEM images and MSV (Morphology Score Vector)

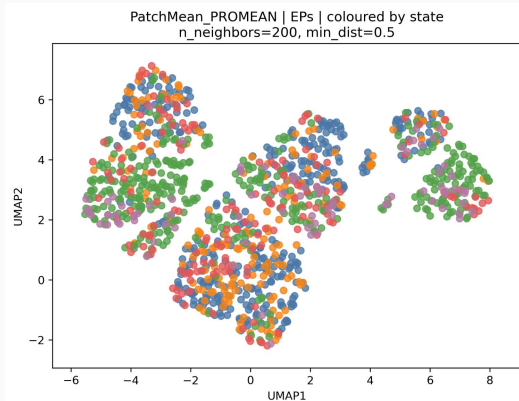
- From **discrete morphology classes** to **continuous scores** — **MSV**:



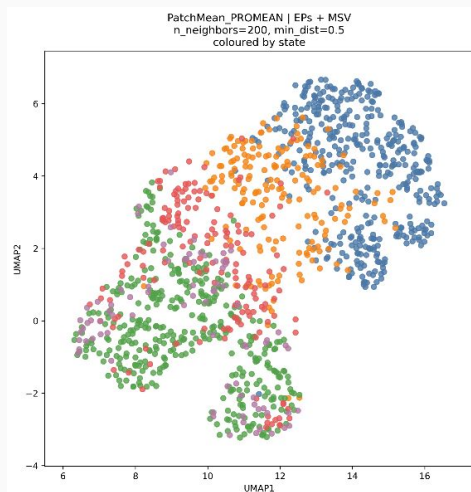
4.4 UMAP Visualisation of Tabular Data + SEM Image Information (MSV)

EPs (coloured by morphology)

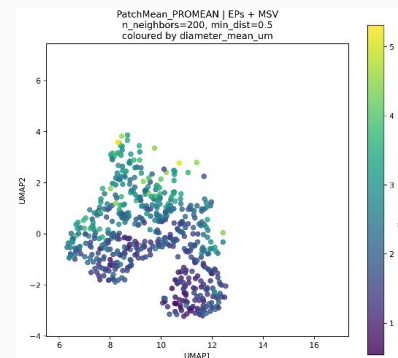
- **EPs (Experimental & Environmental Parameters)**:
concentration, needle gauge, distance, flow rate,
voltage, temperature, humidity



EPs + MSV (coloured by morphology)



EPs + MSV (coloured by diameter)



EPs + MSV (coloured by CV)

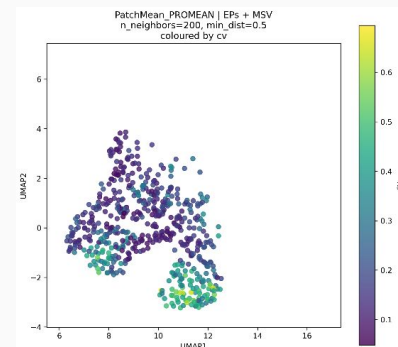


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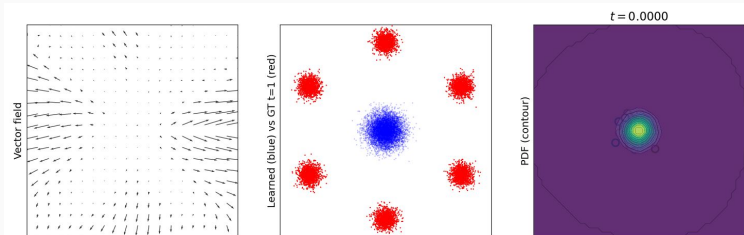
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5.1 Choice of Generative Models

➤ Diffusion and Flow Model (Stable Diffusion, DALL·E, Sora...)

- Mathematical perspective:
Optimal Transport – principled paths between distributions
- Continuous-time dynamics

Flow models – ODE $dX_t = u_t(X_t)dt$



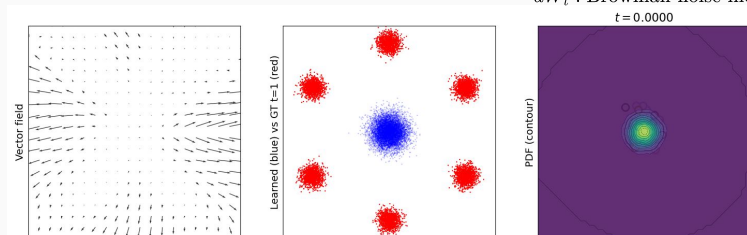
- Numerical Sampling

ODE: Euler method

$$X_{t+h} = X_t + h u_t(X_t)$$

Diffusion models – SDE $dX_t = u_t(X_t)dt + \sigma_t dW_t$

* dW_t : Brownian noise increment



SDE: Euler-Maruyama method

$$X_{t+h} = X_t + h u_t(X_t) + \sqrt{h} \sigma_t \epsilon_t, \\ \epsilon_t \sim \mathcal{N}(0, I)$$



Fig. Left: Progressive generation of a cat image from noise. Right: Conditional generation on a toy dataset with eight Gaussian modes arranged in an octagonal pattern.

5.2 Evaluation of Generated Solutions

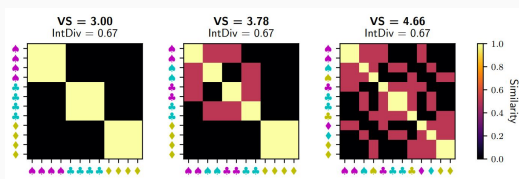
A. Target (Condition) Consistency

$$x_i \xrightarrow{\text{forward surrogate}} \hat{y}_i$$
$$\hat{y}_i \stackrel{?}{\approx} y^*$$

B. Solution Diversity

$$c = c^*, \quad x_1, \dots, x_N \sim p_\theta(x|c^*)$$

- Generate multiple candidates for a fixed target
→ Quantify solution diversity (e.g. **Vendi Score**)

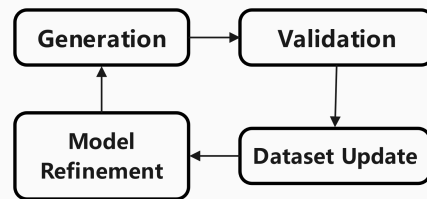


C. Target-Neighbourhood Evaluation

$$\bigcup_{c \in \mathcal{N}(c^*)} p(x | c)$$

- Explore solutions over an acceptable target range
→ Expand the feasible solution space
→ Assess local conditional smoothness

D. Experimental Validation and Model Refinement



5.3 Expected delivery: (Calibrated) Estimate of Solution Reliability

- Given a recommended candidate:

$$x^* = [C, Q, V, L, G]$$

- How **reliable** is this candidate?
 - Candidate-specific calibrated prediction intervals
 - Using for example **Conformalized Quantile Regression (CQR)**
 - **Example:**

Candidate A

Recommended recipe: x_A^*

Expected diameter: **0.85–1.05 μm**

Expected CV: **< 0.20**

Confidence level: 95%

Thank you for your attention!

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