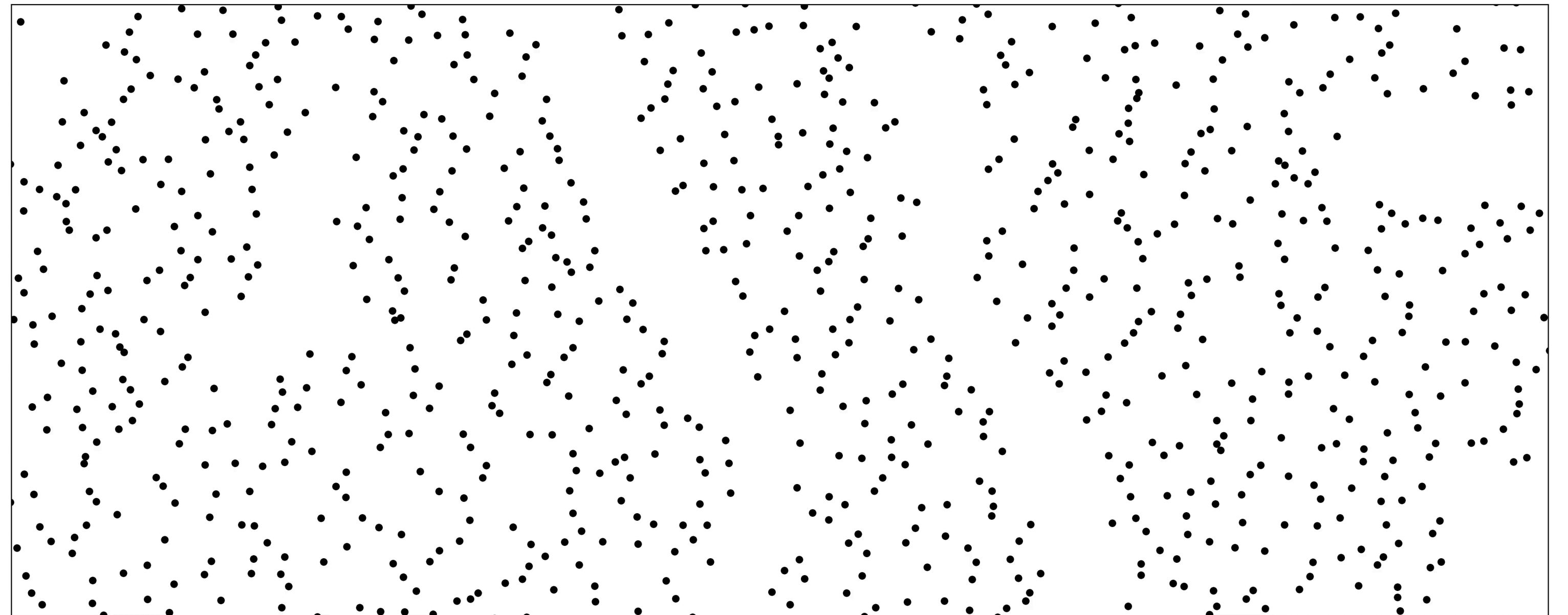
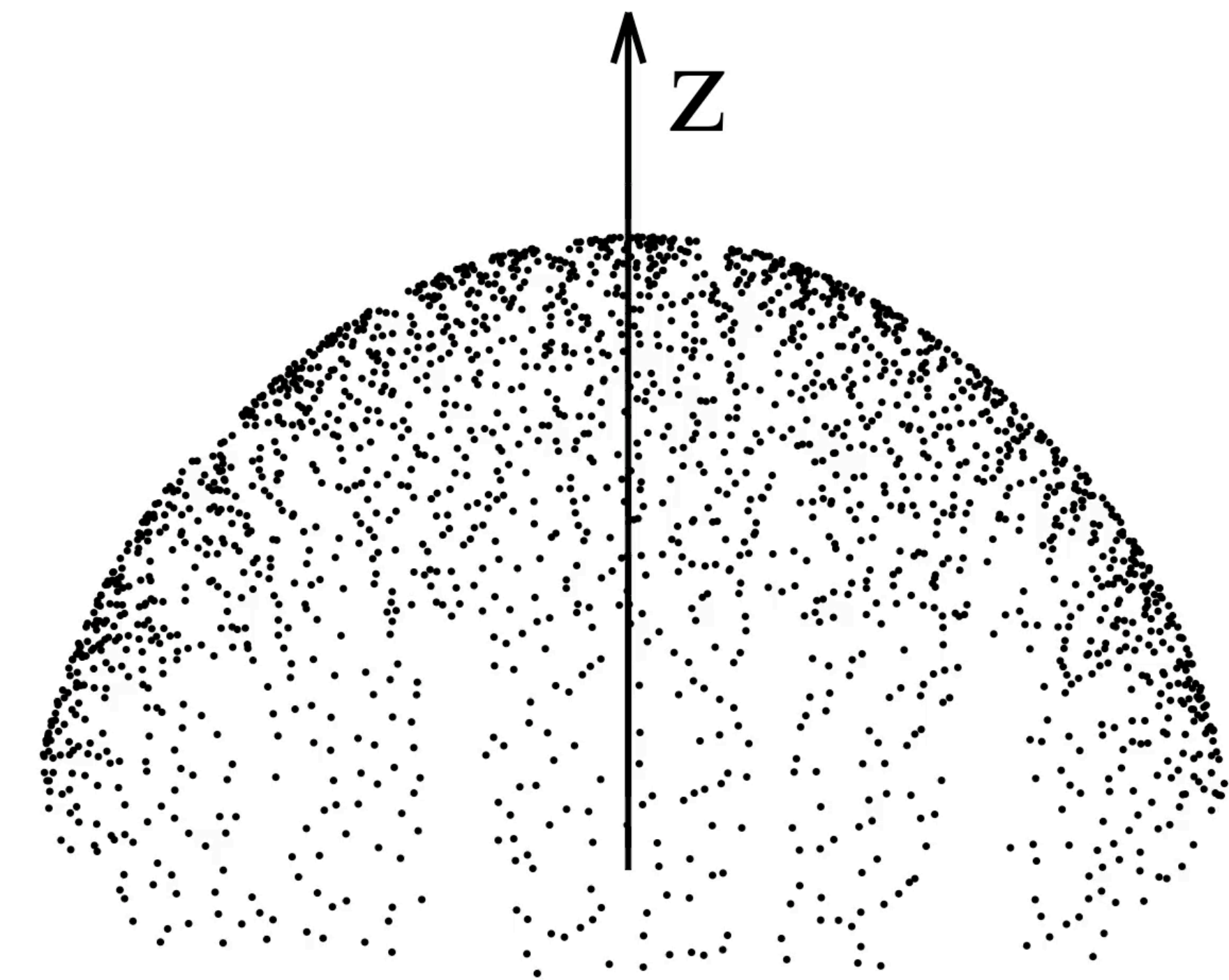


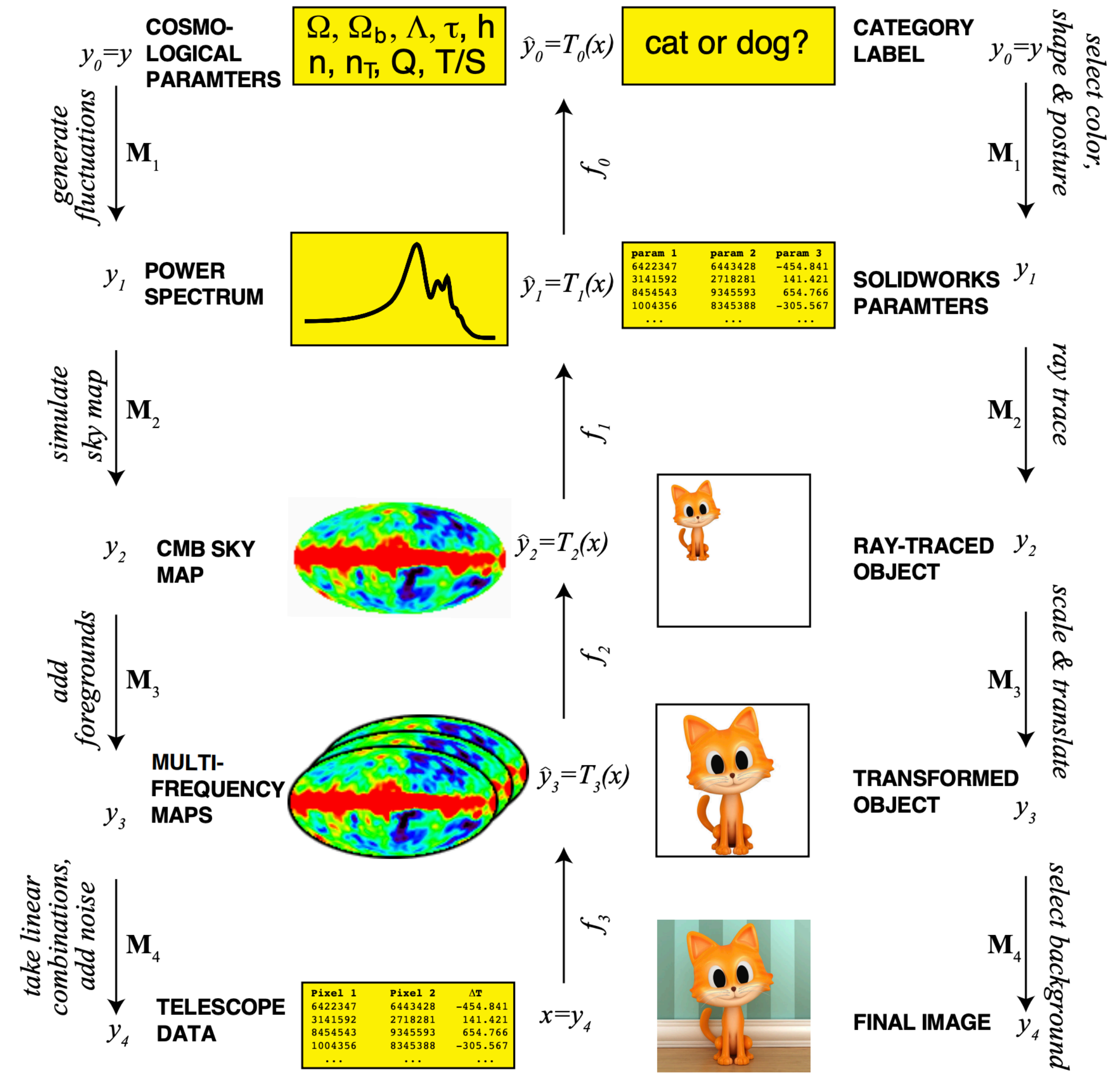
From Physics to Generative Models



Ziming Liu, IAIFI Journal Club, April 18 2023
Advisor: Max Tegmark

Q: Can physics help build generative models?

Our Universe/Physics is a generative model



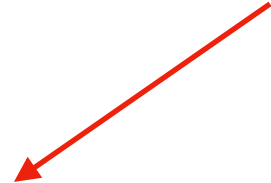
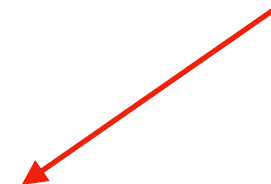
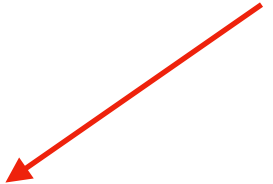
Thank you for your listening!

~~**Thank you for your listening!**~~

Just kidding!

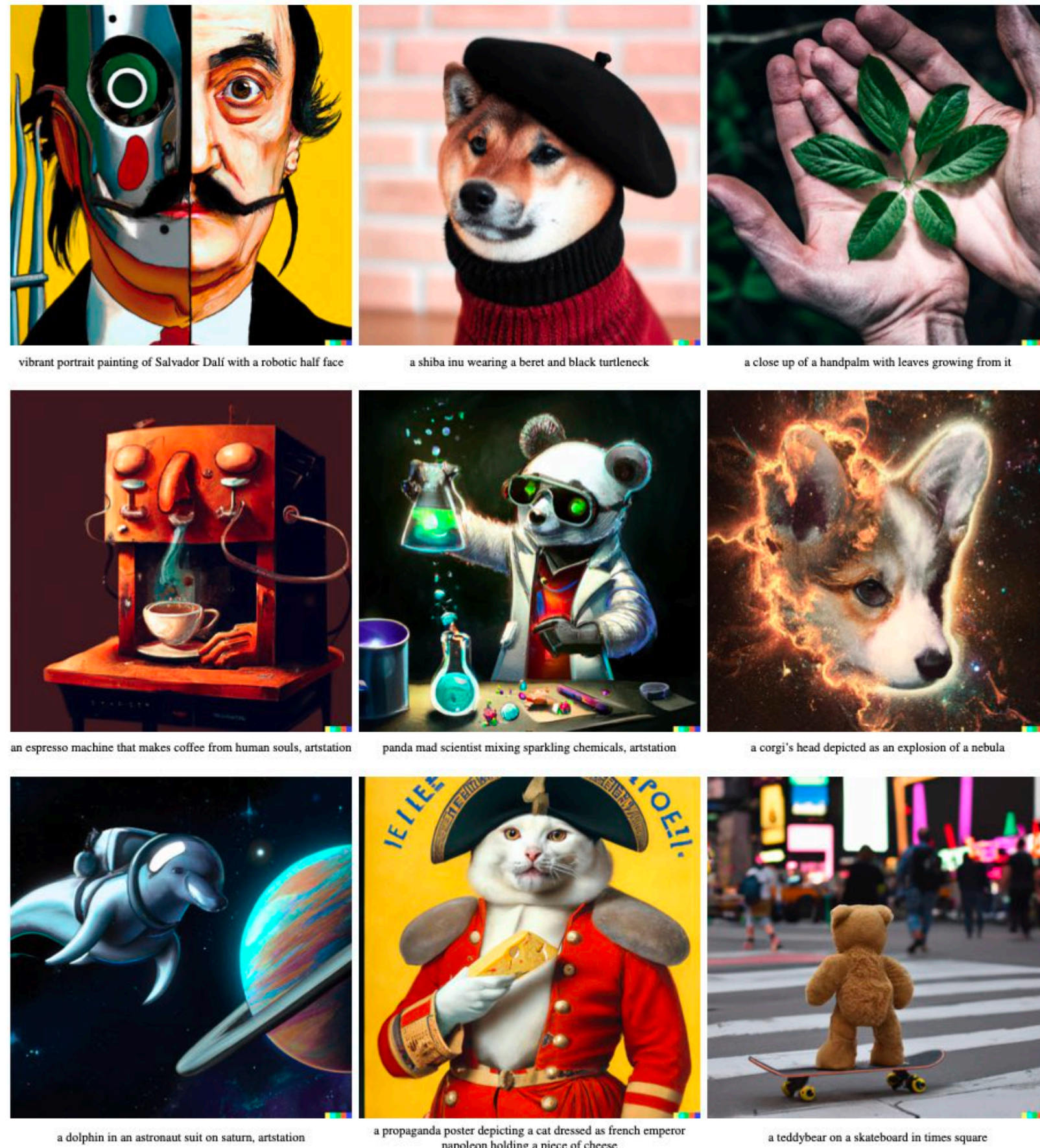
Need actually build generative models!

Overview

1. Brief background: Diffusion Models (DM)  Diffusion process
2. Poisson flow generative models (PFGM/PFGM++)  Electrostatics
3. GenPhys: From Physical Processes to Generative Models  Any physical process?

Generative Models

DALLE-2

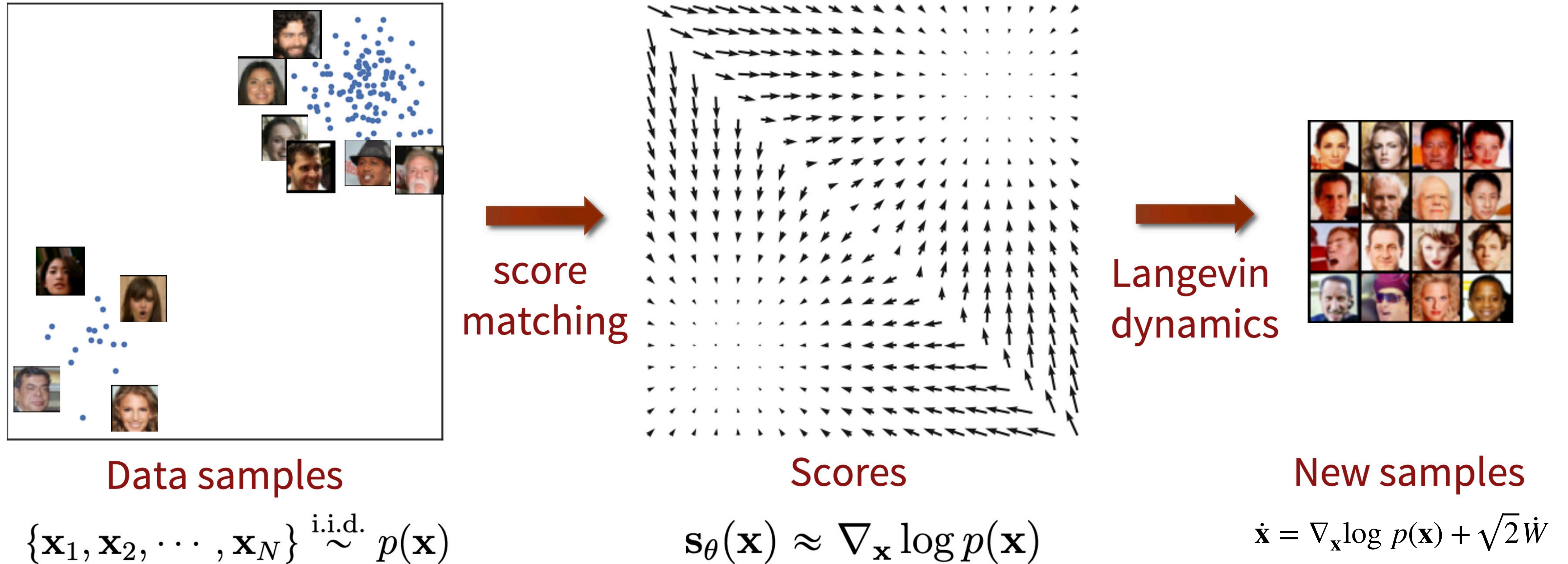


Stable diffusion



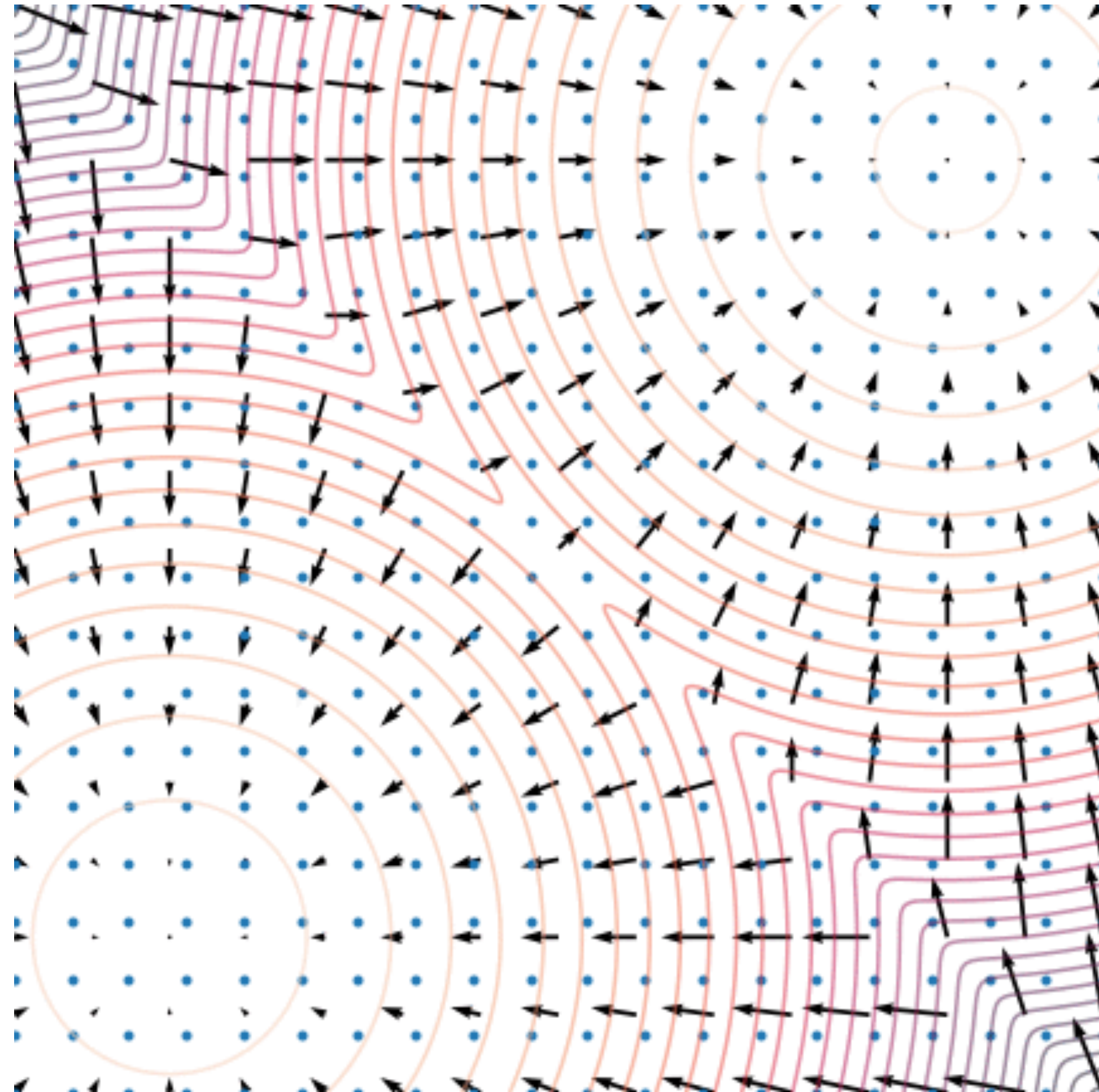
Figure 1: Selected 1024×1024 samples from a production version of our model.

Score-based models (diffusion models)



Physics interpretation $p(\mathbf{x}) = \exp(-E(\mathbf{x}))$ $\mathbf{s}_\theta(\mathbf{x}) = -\nabla E(\mathbf{x})$

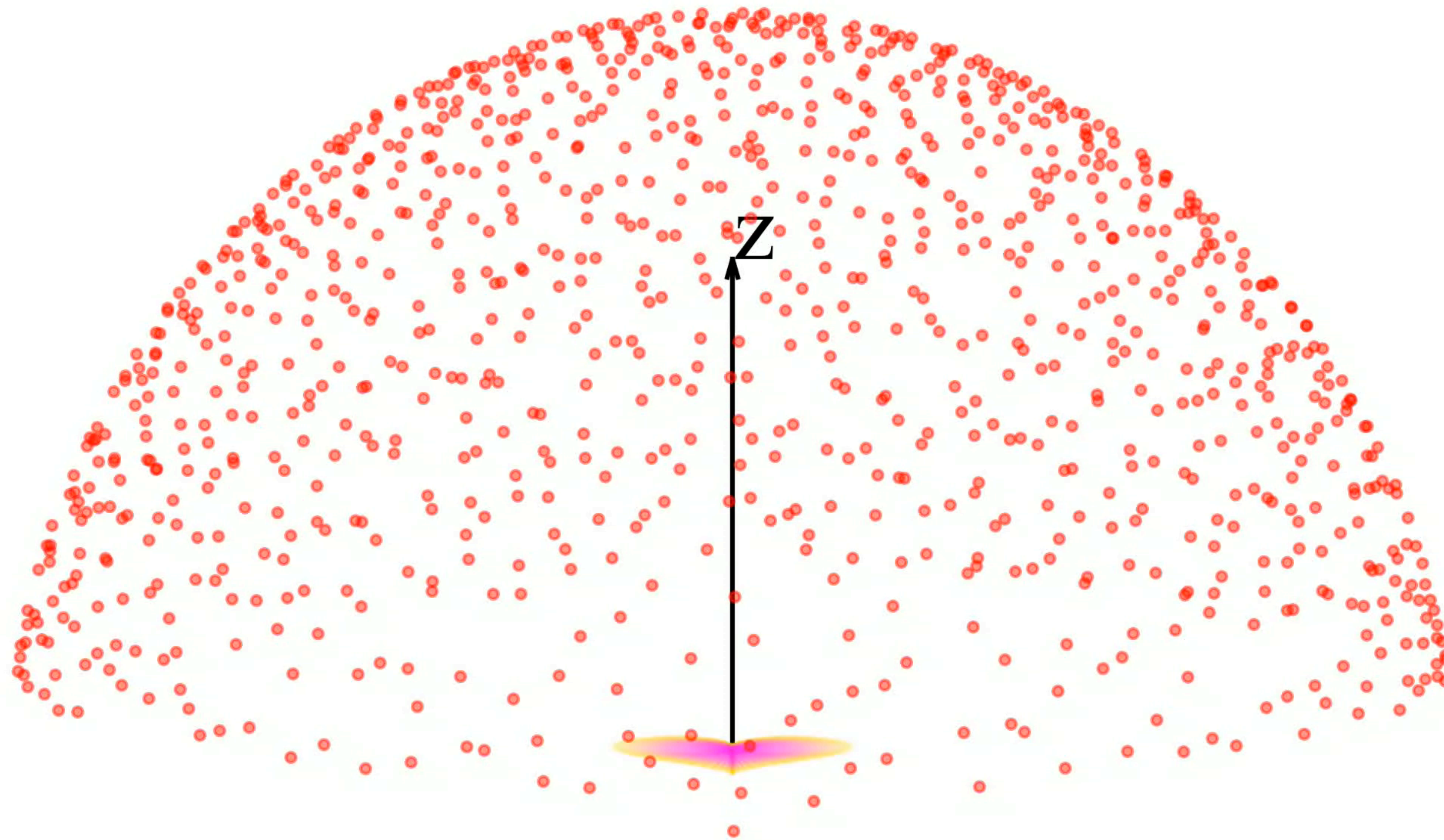
Score-based models (diffusion models)



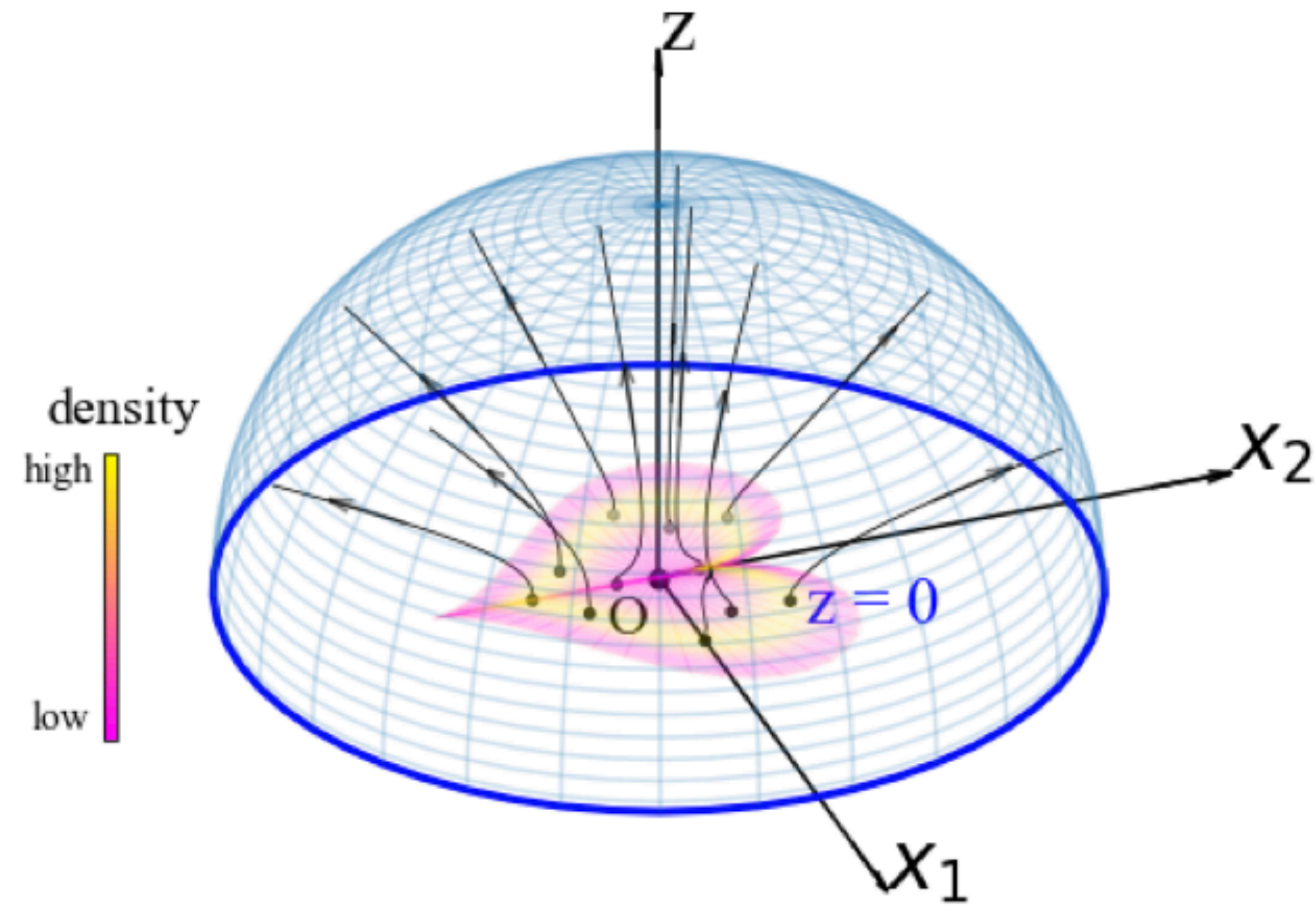
Poisson Flow Generative Models

Yilun Xu*, Ziming Liu*, Max Tegmark & Tommi Jaakkola

Accepted by NeurIPS 2022



Basic idea

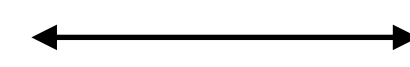


Generative modeling



Physics

data point/sample



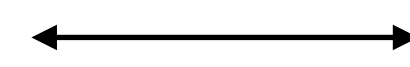
electric charge

data distribution



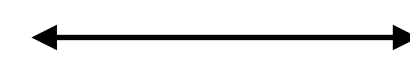
charge distribution

flow



electric field/flux

bijection map



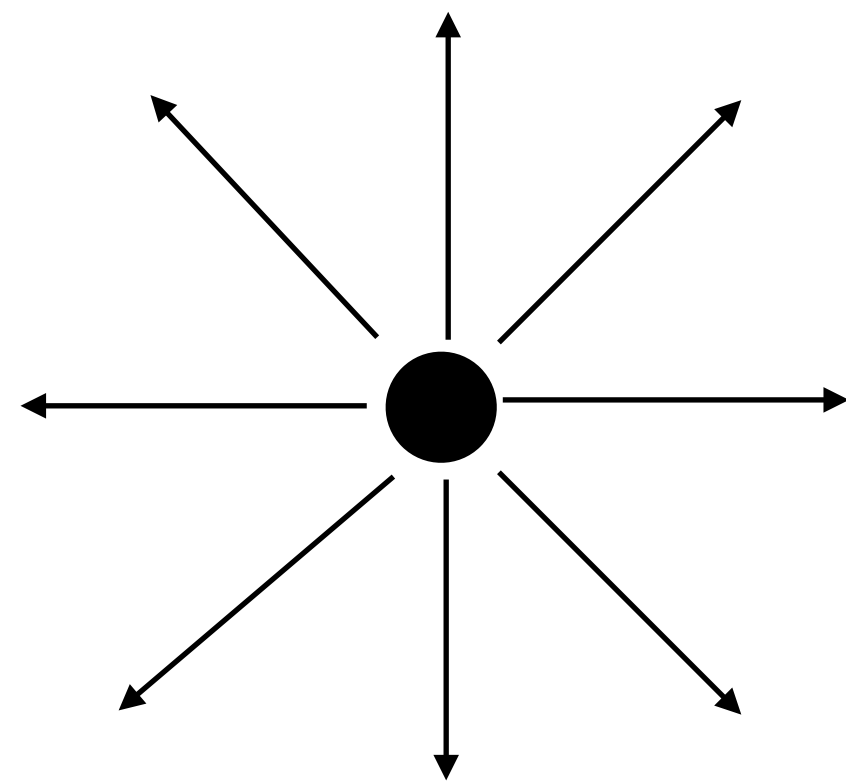
electric lines

Electrostatics

Poisson Equation $\nabla^2 \varphi = -\rho(x)$, $\nabla^2 \equiv \sum_{i=1}^N \partial_i^2$

Green function $\nabla^2 G(x, x') = -\delta(x - x') \implies G(x, x') \sim r^{-(N-2)}$, $r \equiv ||x - x'||$

$$\varphi(x) = \int G(x, x') \rho(x') dx' \quad E(x) = -\nabla \varphi(x) \sim \int \frac{x - x'}{||x - x'||^N} \rho(x') dx'$$



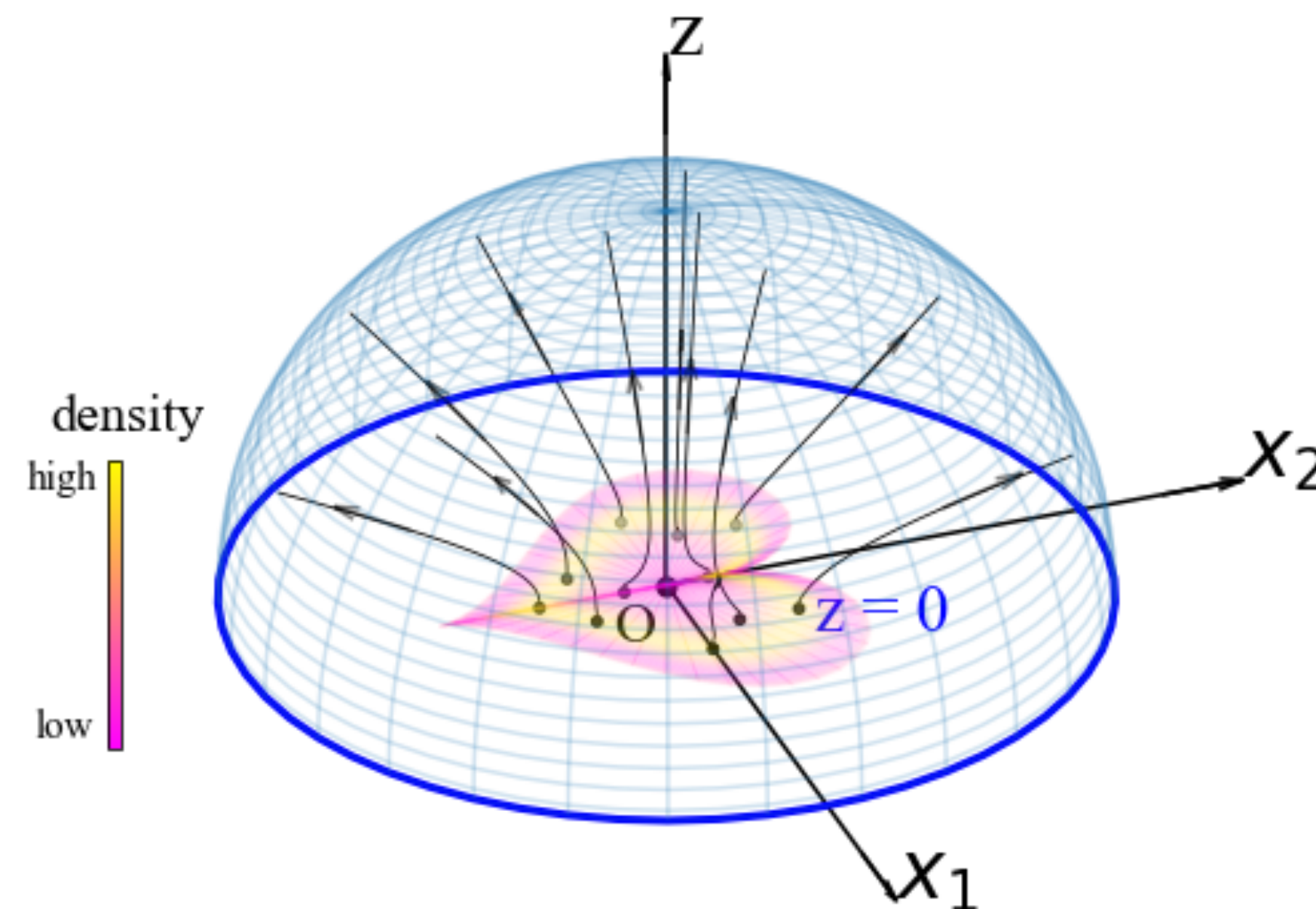
$$N = 3 \implies \varphi(r) \sim \frac{1}{r}, E(r) \sim \frac{1}{r^2}$$

$$N \geq 3 \implies \varphi(r) \sim \frac{1}{r^{N-2}}, E(r) \sim \frac{1}{r^{N-1}}$$

Electric field
↓ generalize
Poisson field

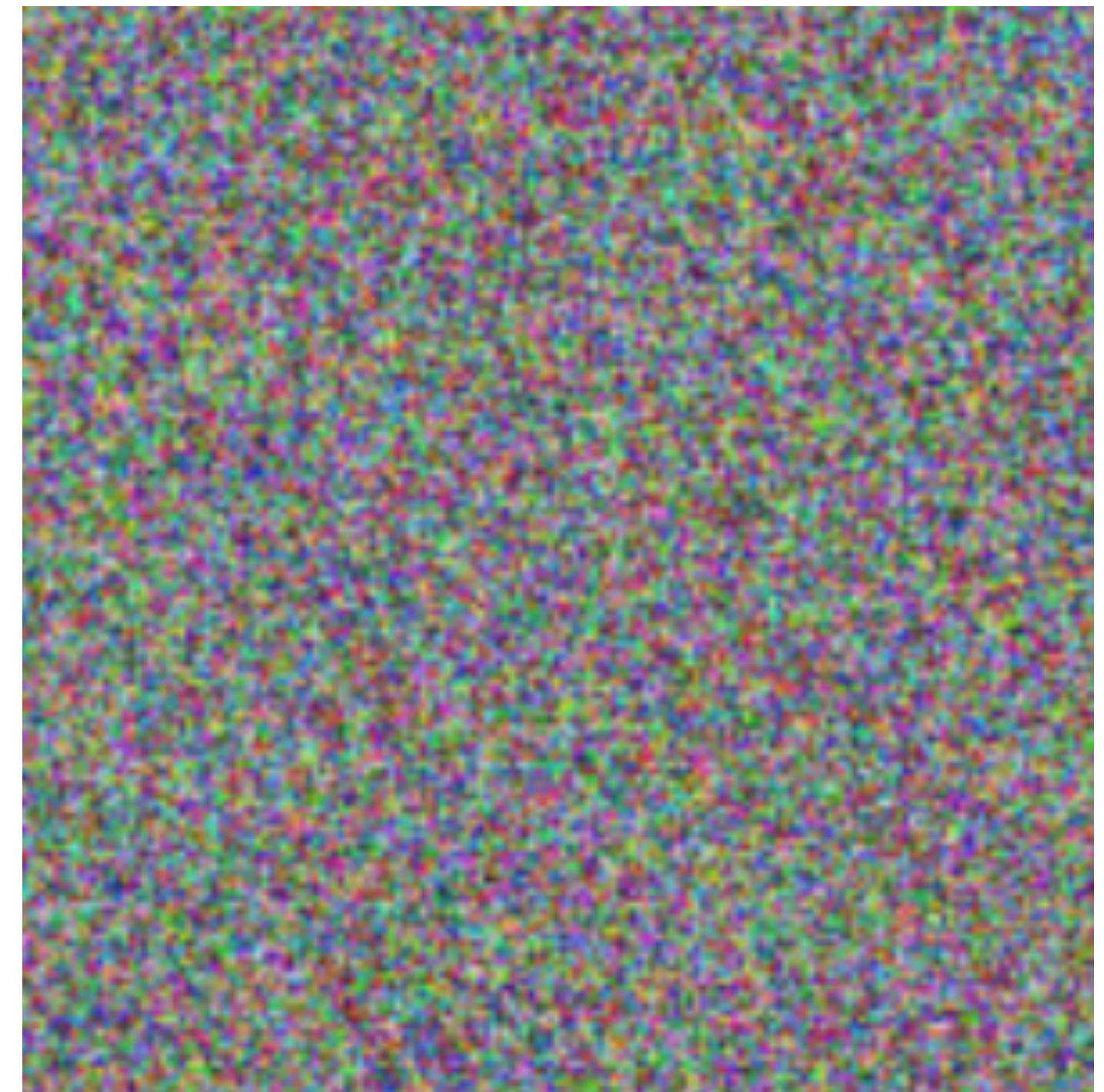
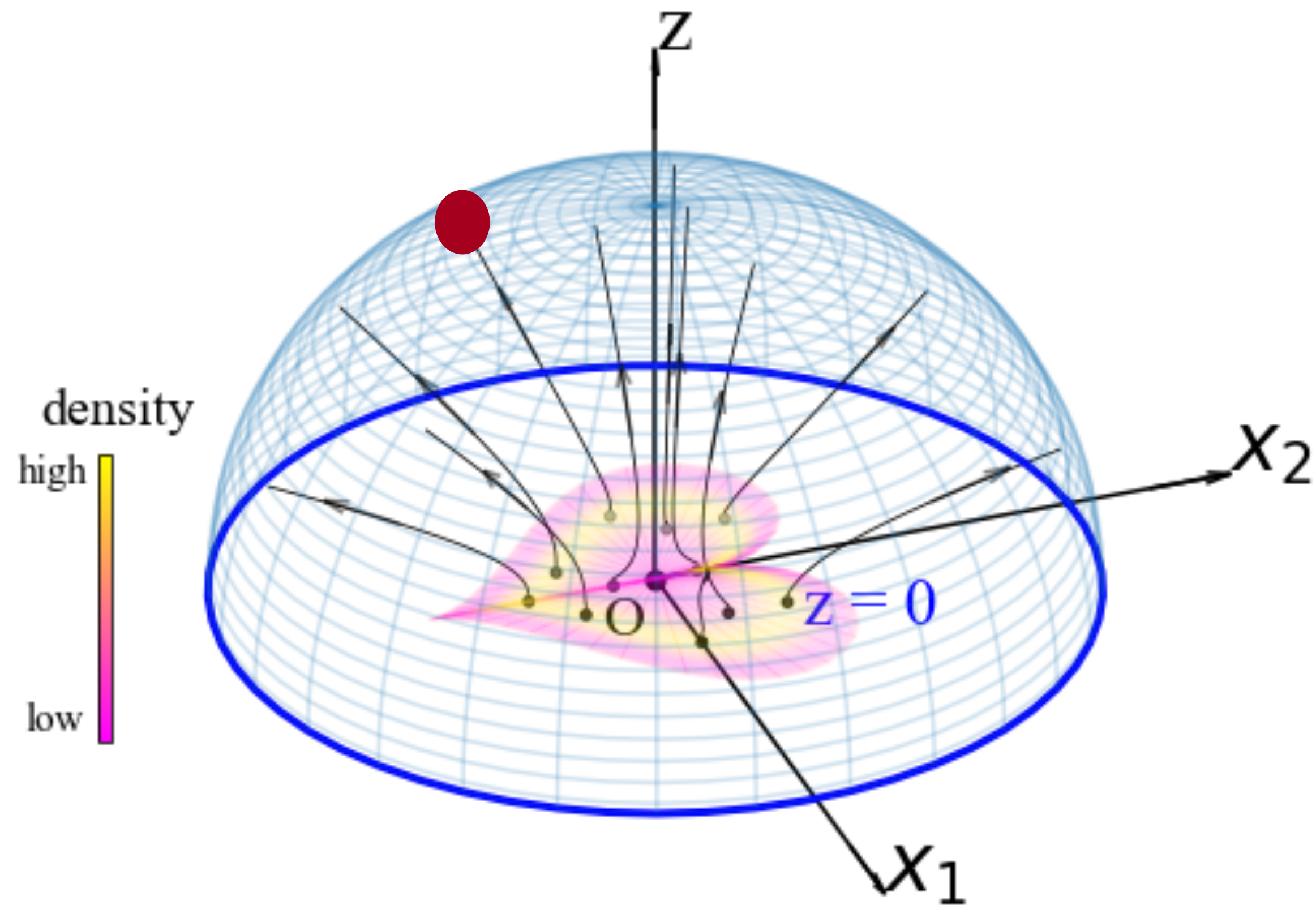
Poisson Flow: a New Flow Inspired by Electrostatics

- Interpret N -dim **data distribution** as **charge density**
- Placing the charges on the $\mathbf{z} = \mathbf{0}$ hyperplane in an $N + 1$ -dim space augmented with dimension \mathbf{z}
- Electric Field Lines *define a bijection* between *data distribution* and a *uniform distribution on the large hemisphere*



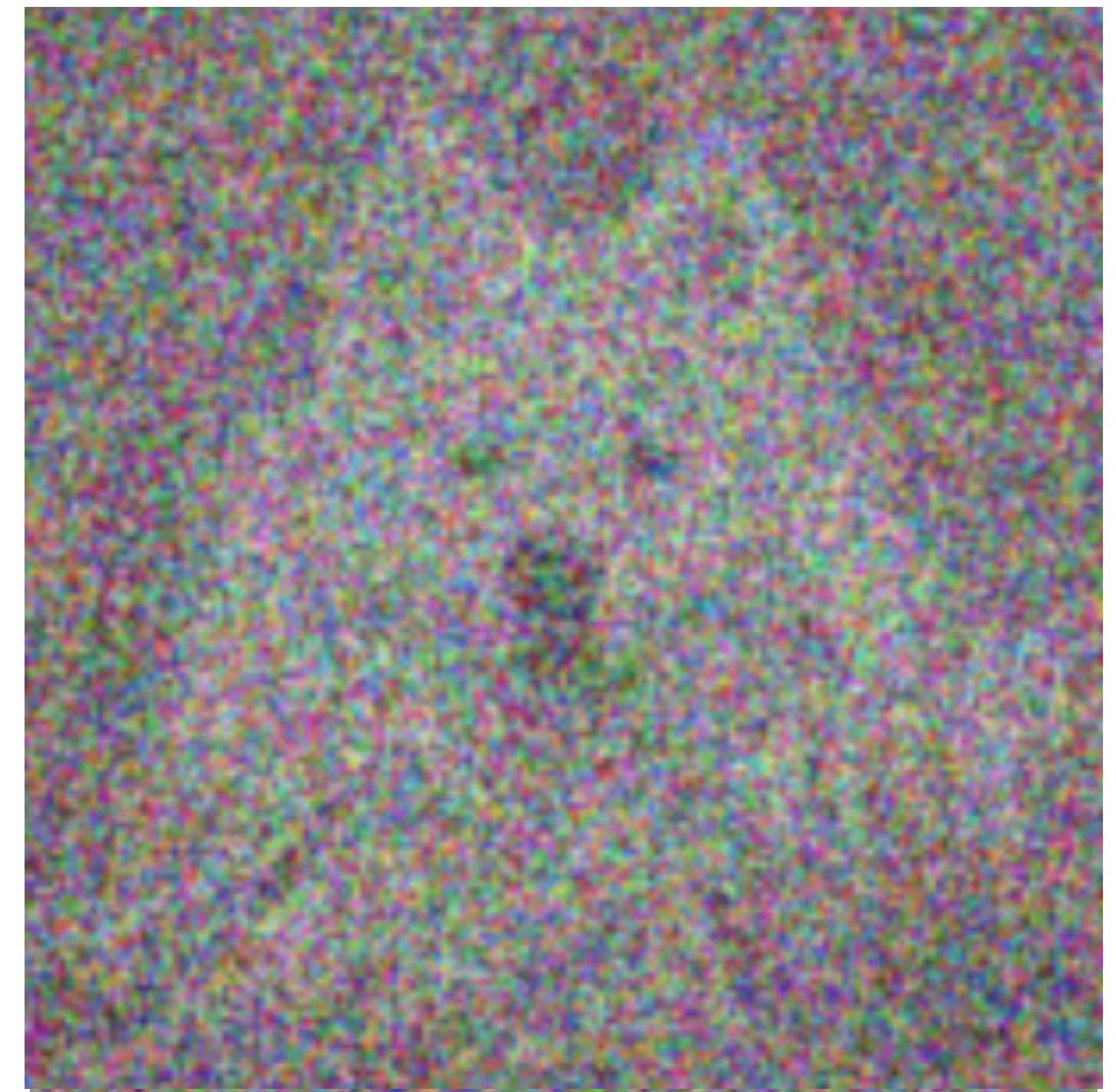
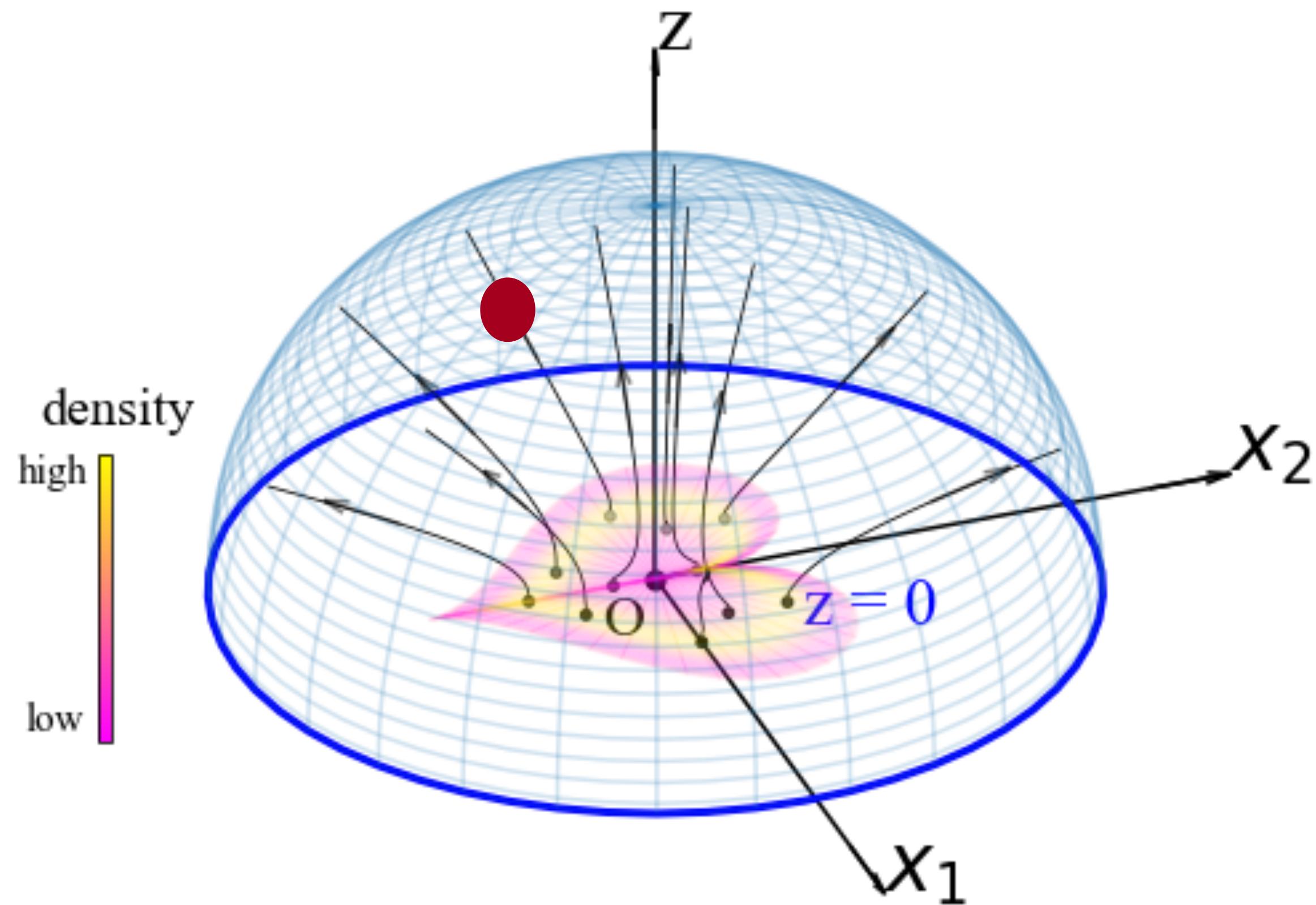
Generation

1. Uniformly sampling an initial sample (●) on the hemisphere.



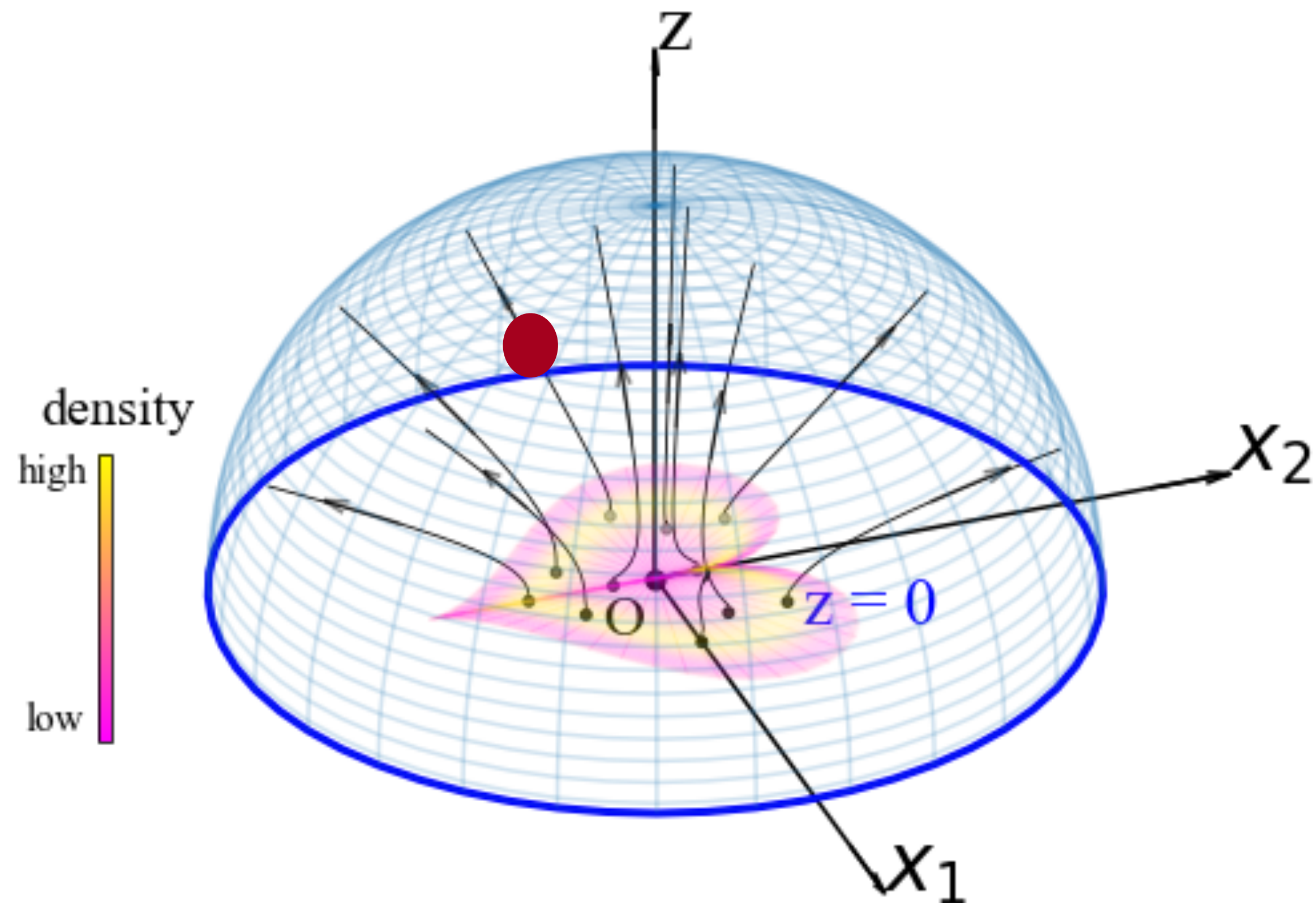
Generation

1. Uniformly sampling an initial sample (●) on the hemisphere.
2. Evolving the sample by following the corresponding electric field line.



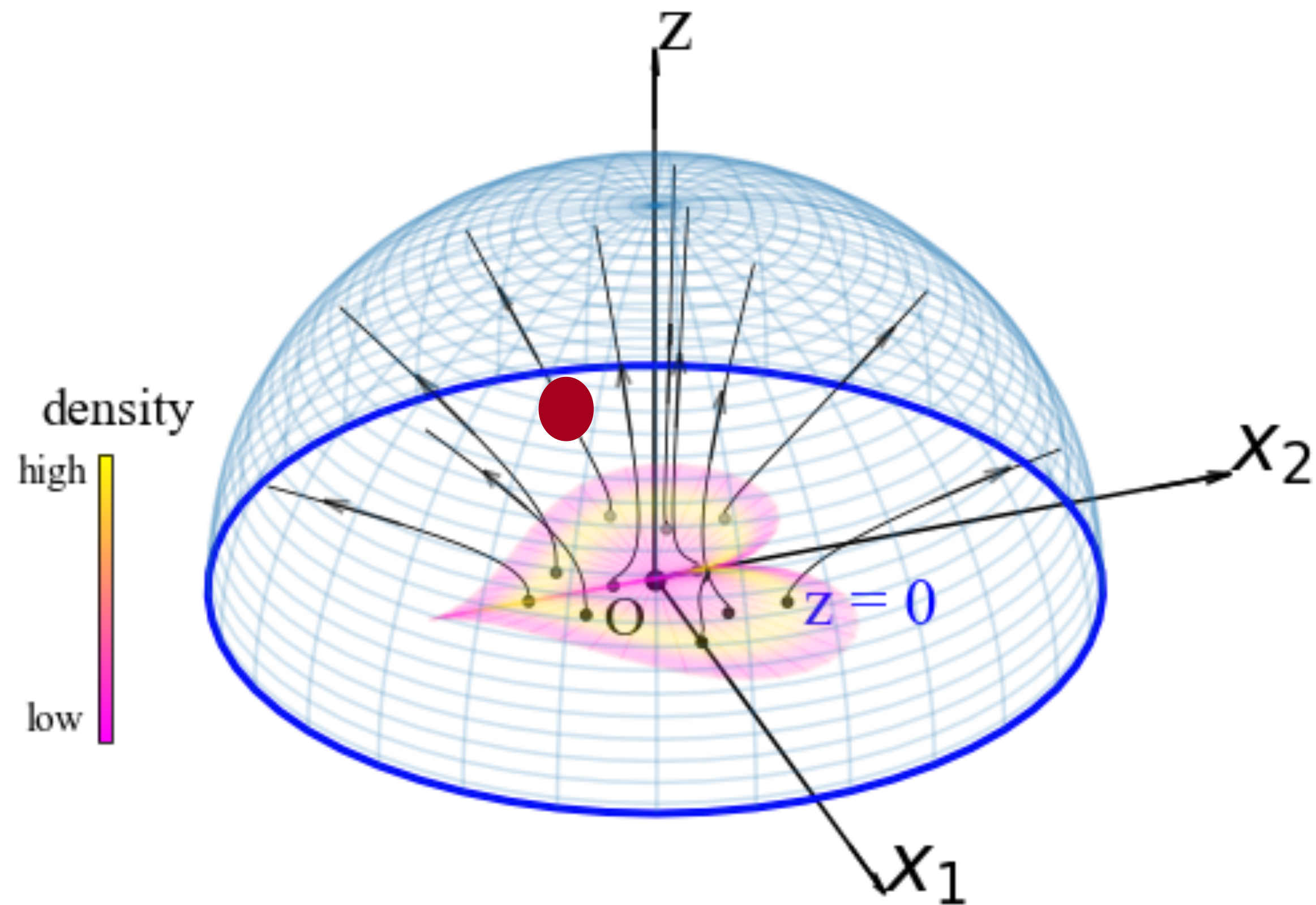
Generation

1. Uniformly sampling an initial sample (●) on the hemisphere.
2. Evolving the sample by following the corresponding electric field line.



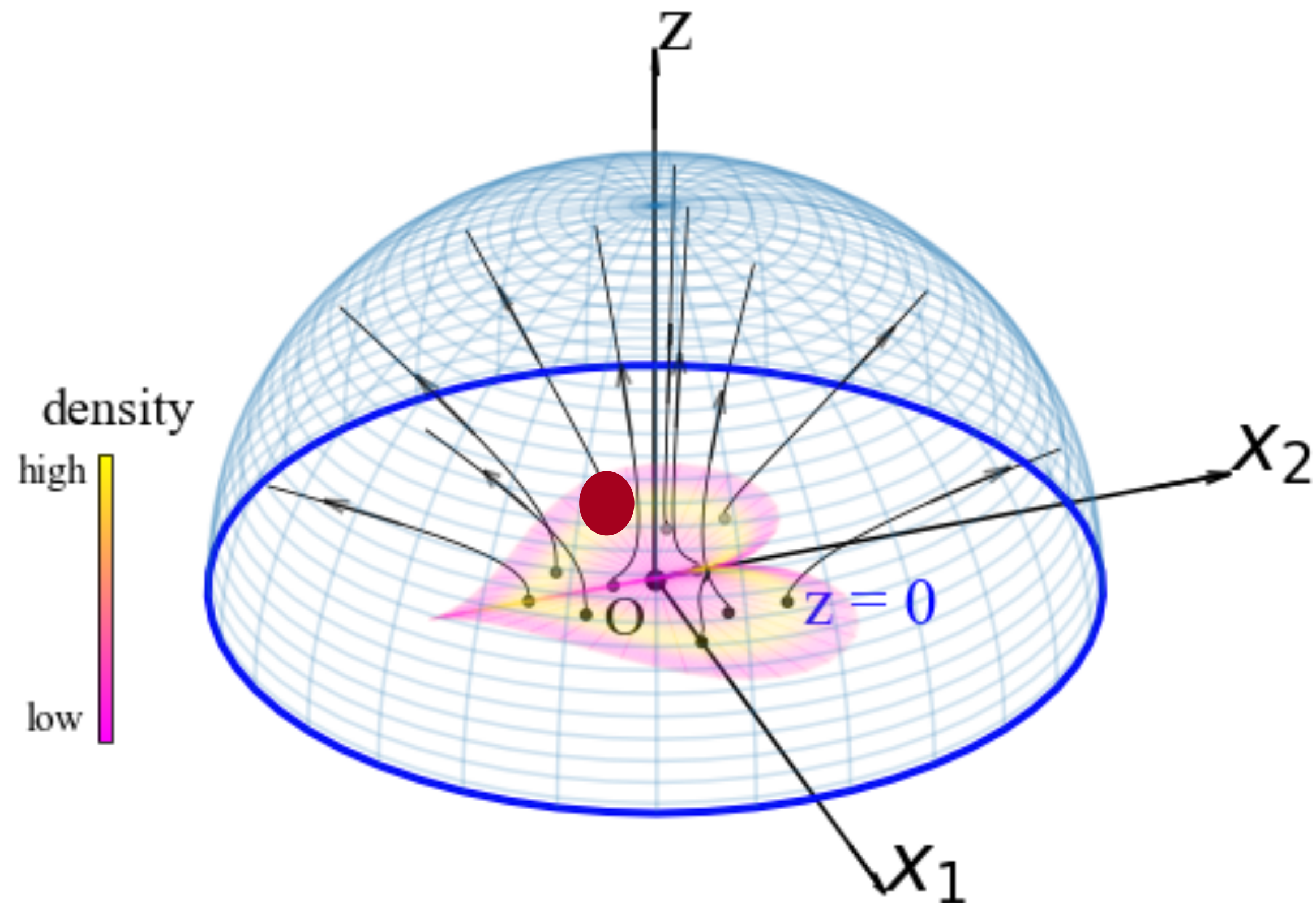
Generation

1. Uniformly sampling an initial sample (●) on the hemisphere.
2. Evolving the sample by following the corresponding electric field line.

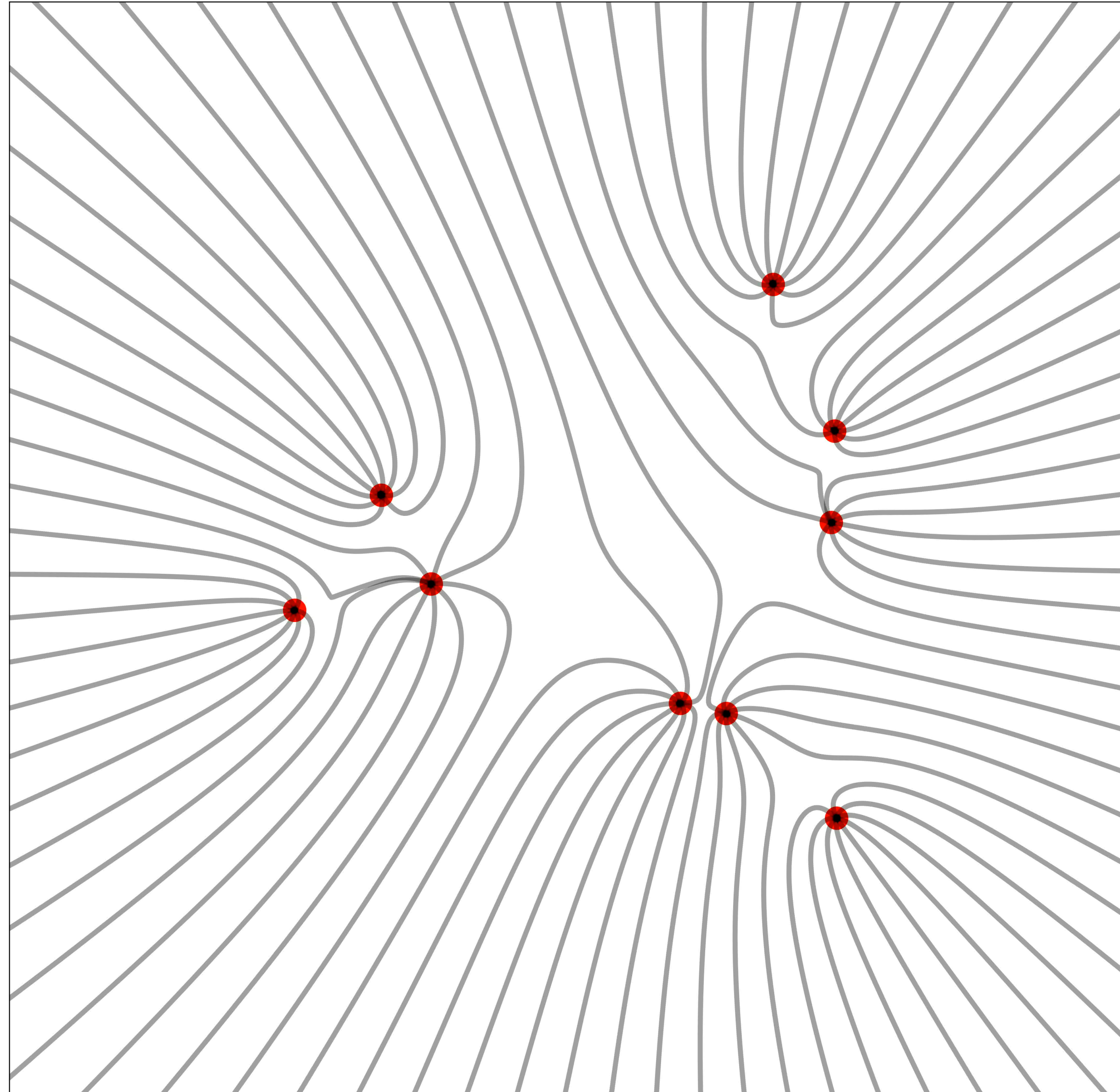


Generation

1. Uniformly sampling an initial sample (●) on the hemisphere.
2. Evolving the sample by following the corresponding electric field line.
3. Stopping the process when $z = 0$.

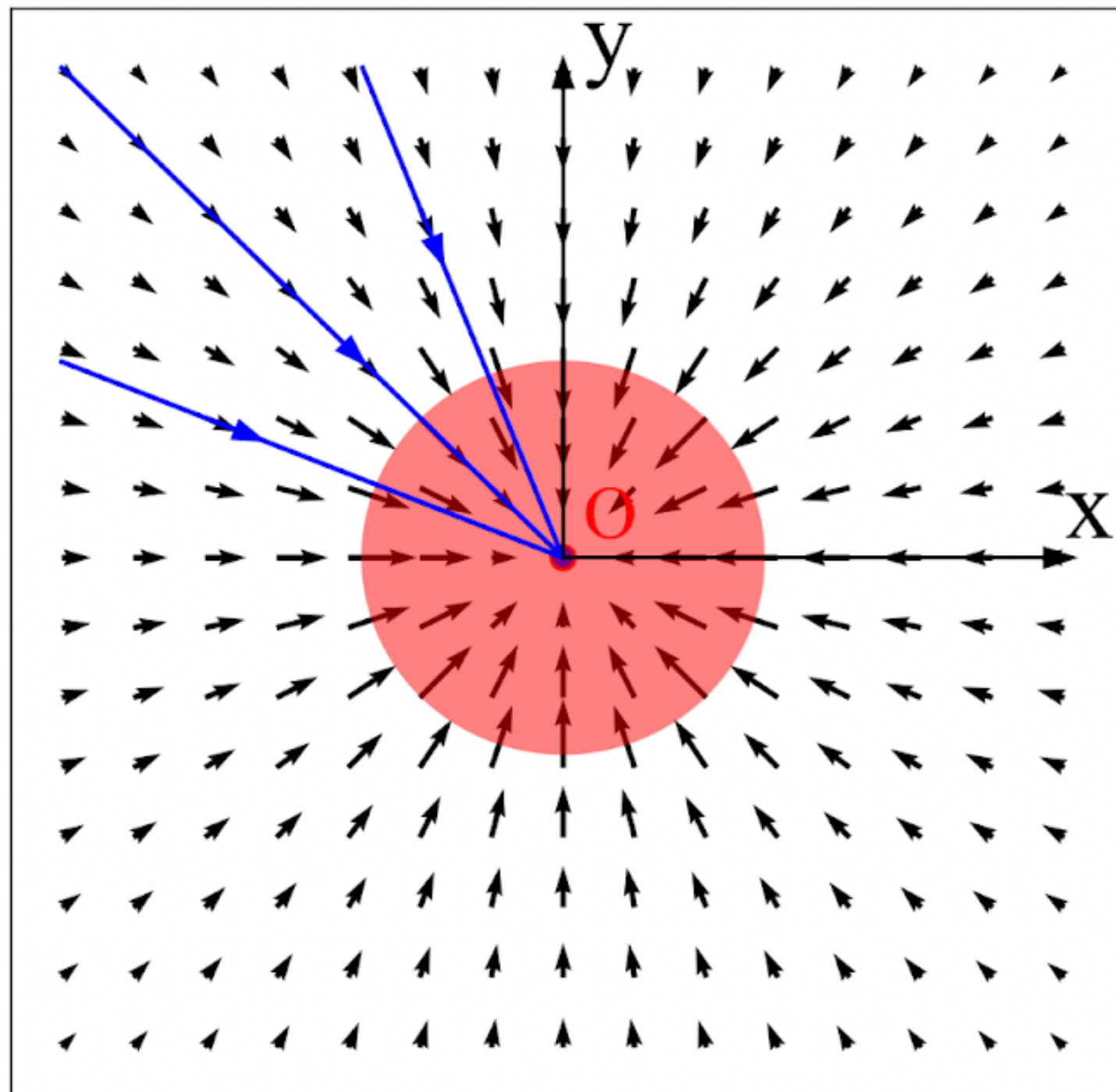


Why bijection?

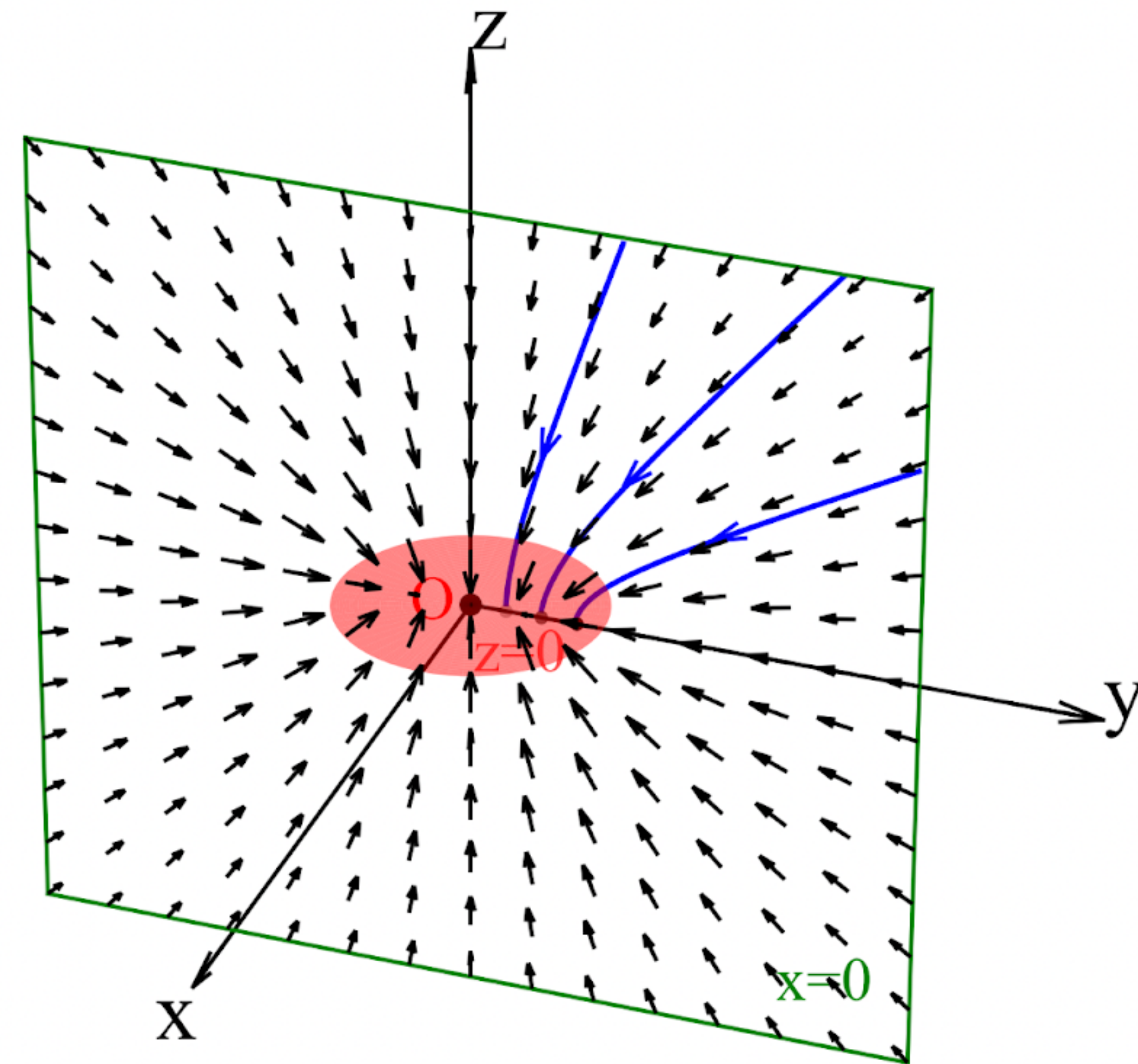


Why augmentation?

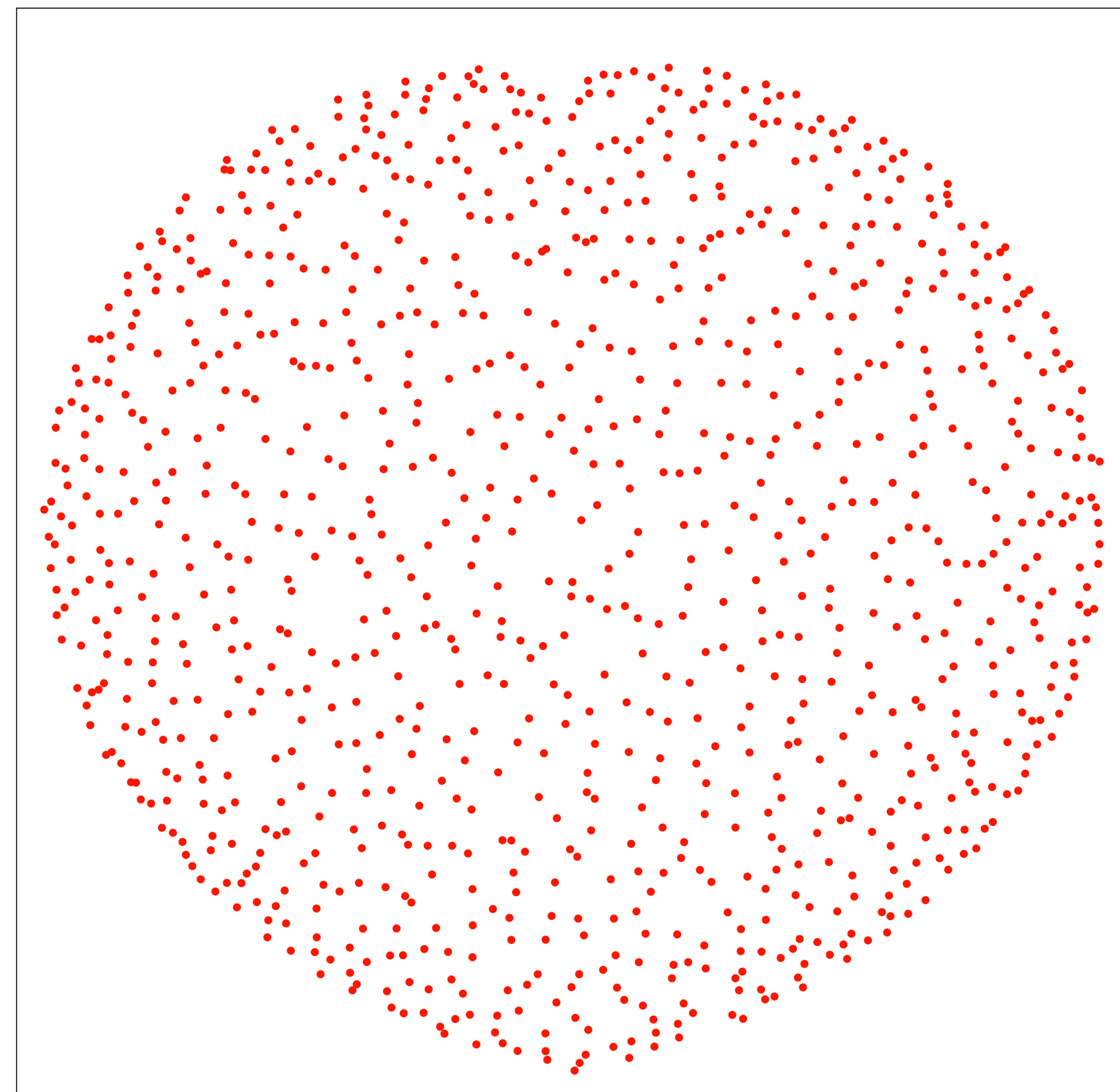
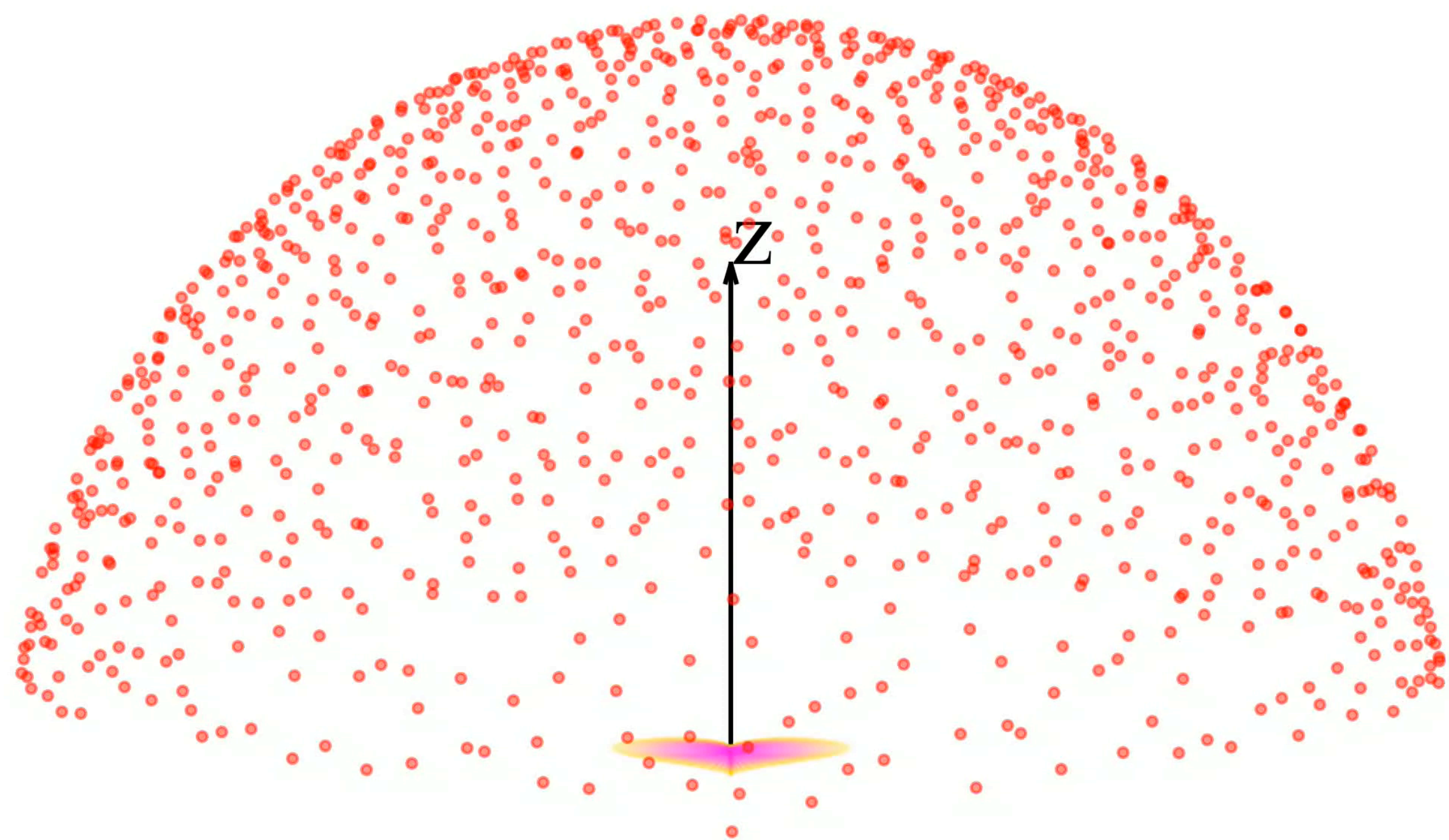
No augmentation (2D)



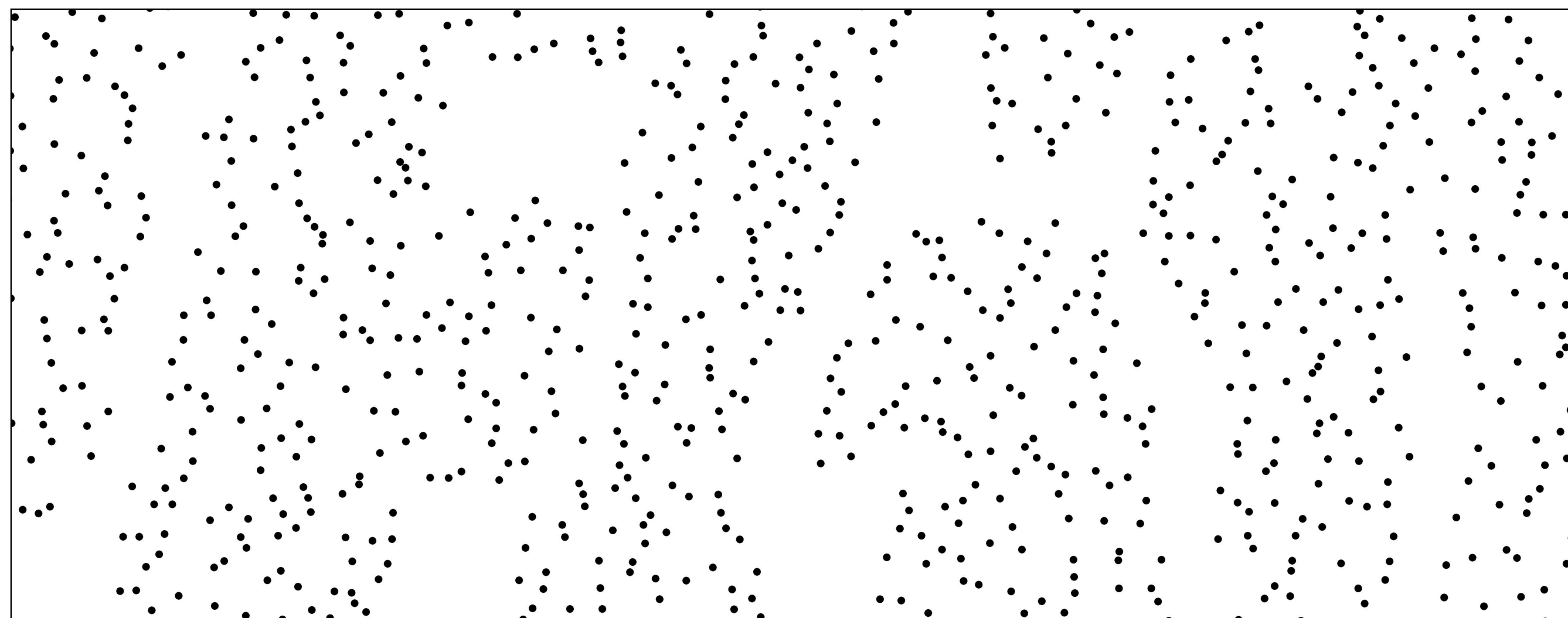
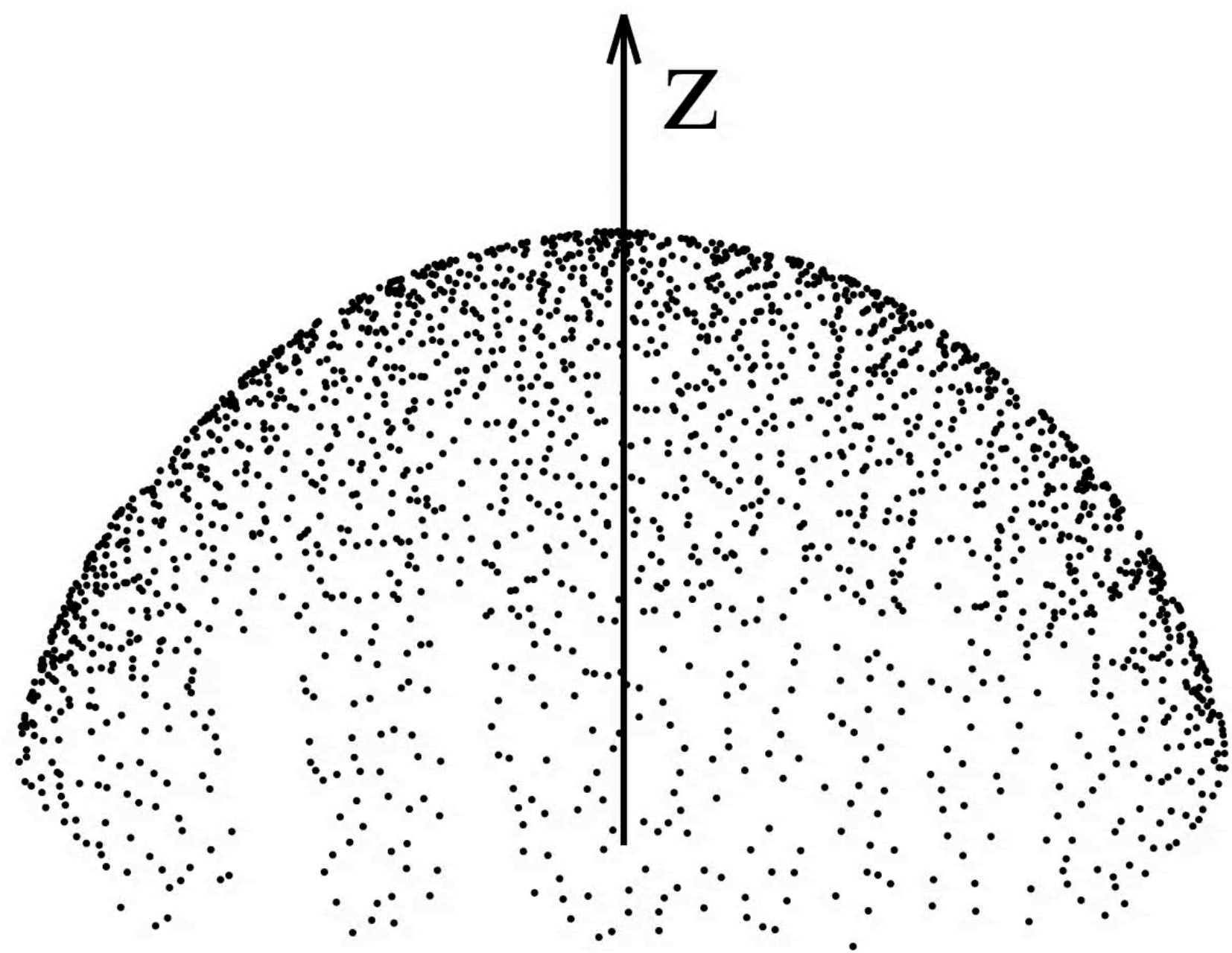
Augmentation (3D)



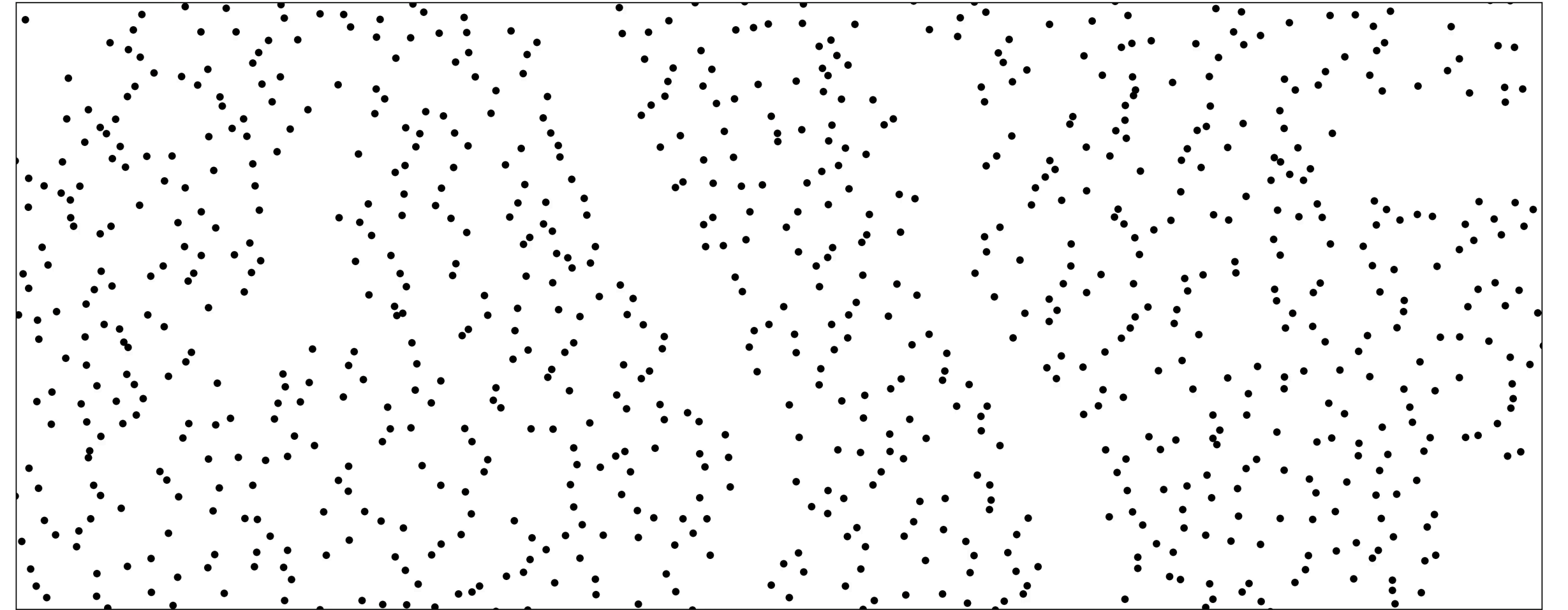
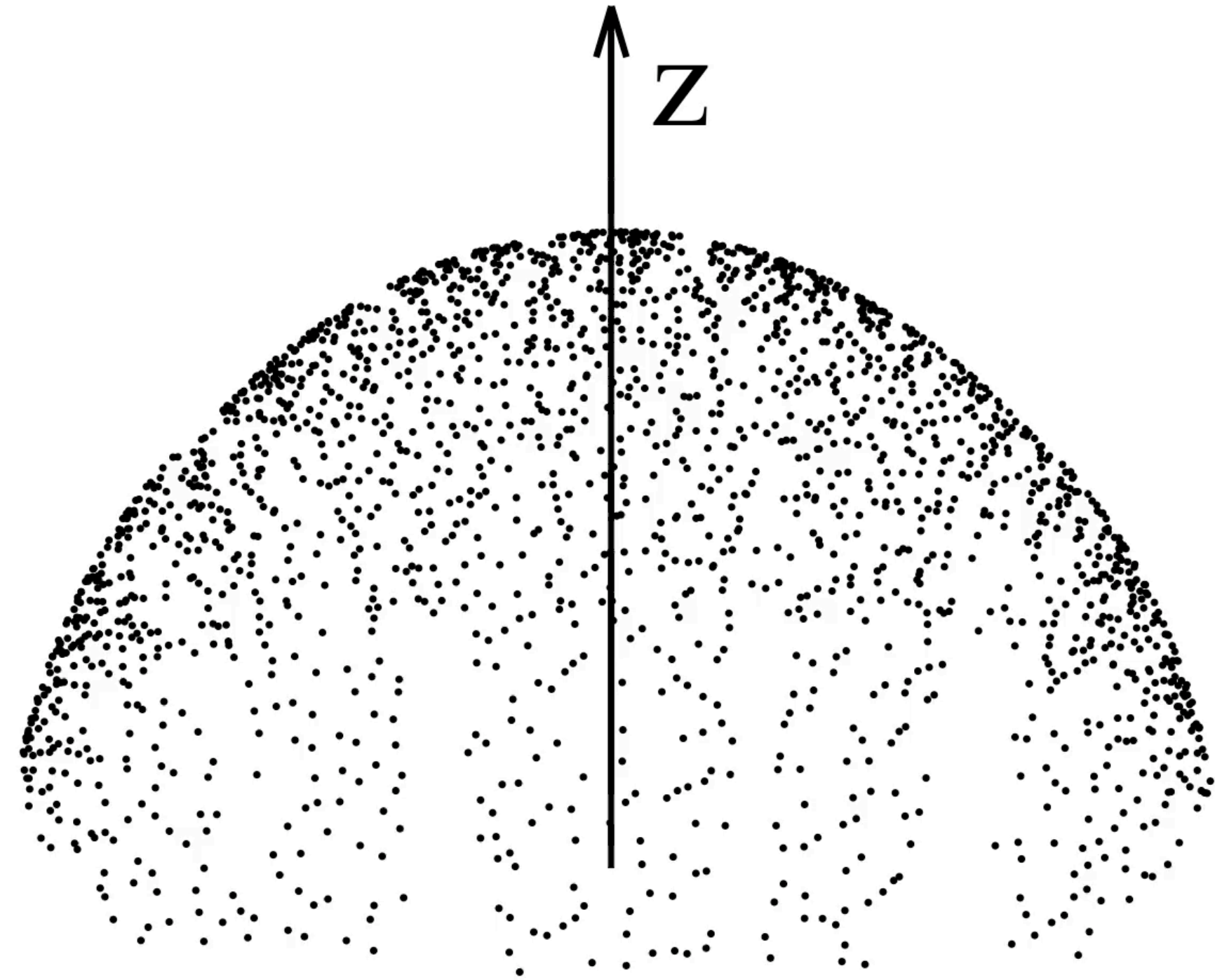
Demo (Heart)



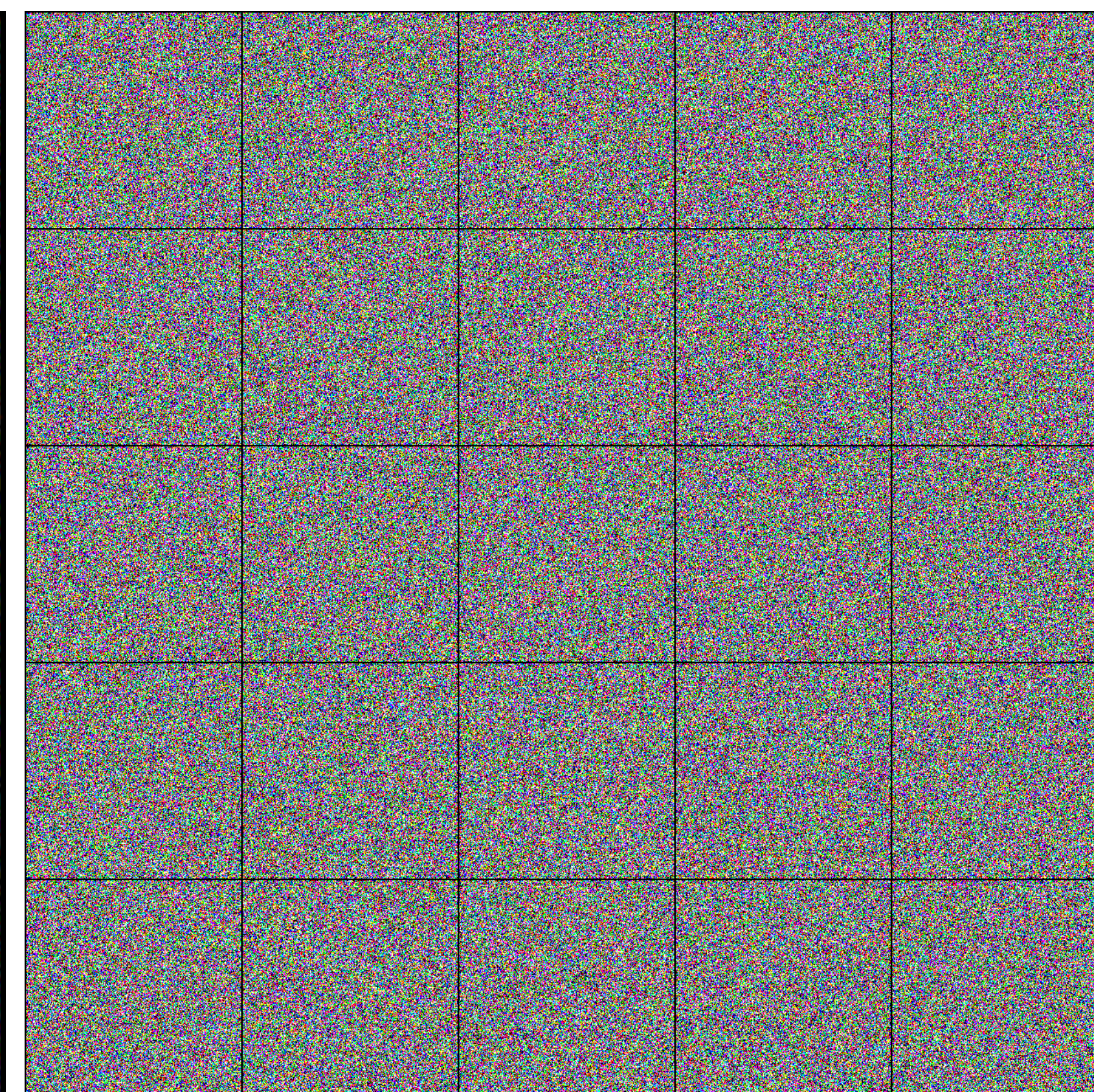
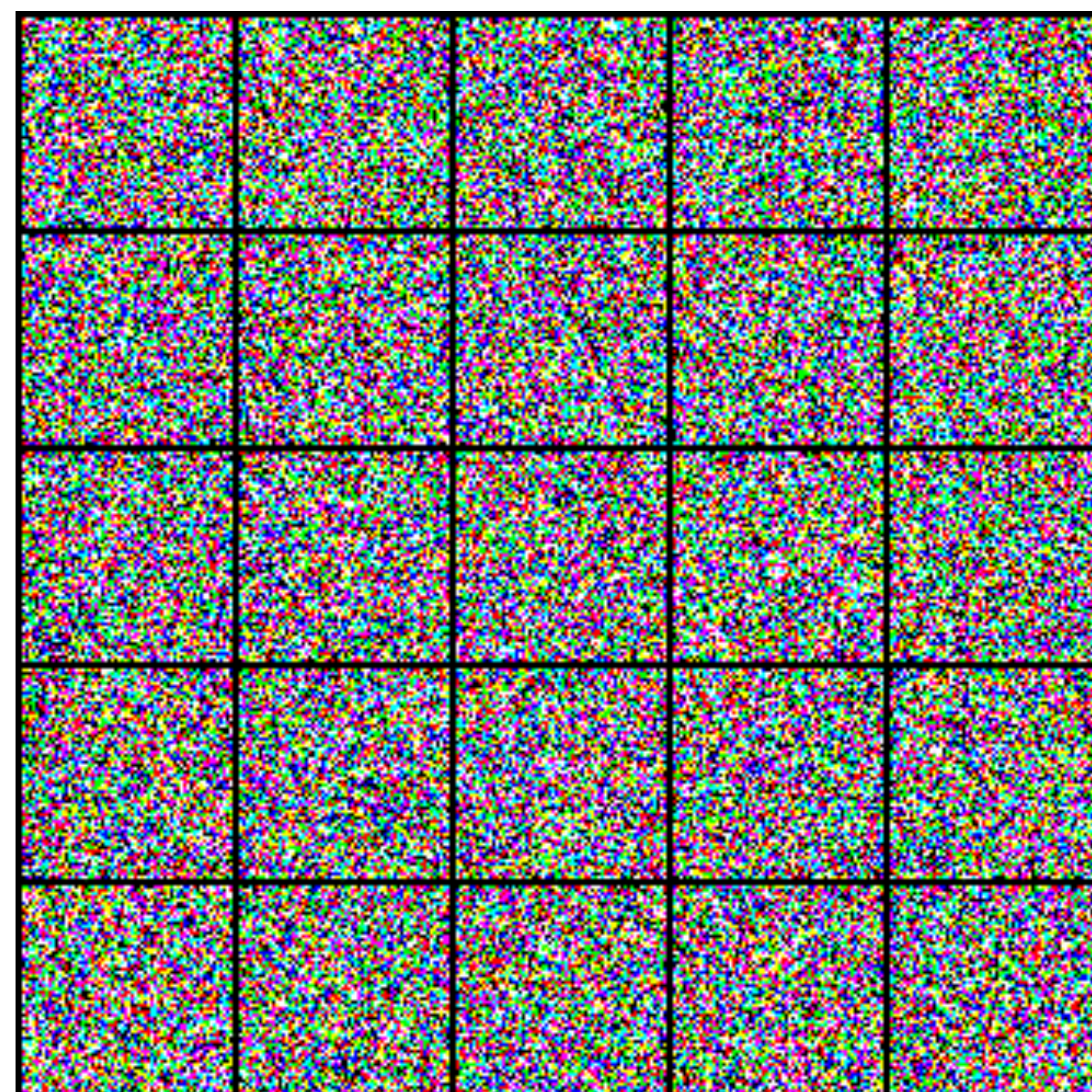
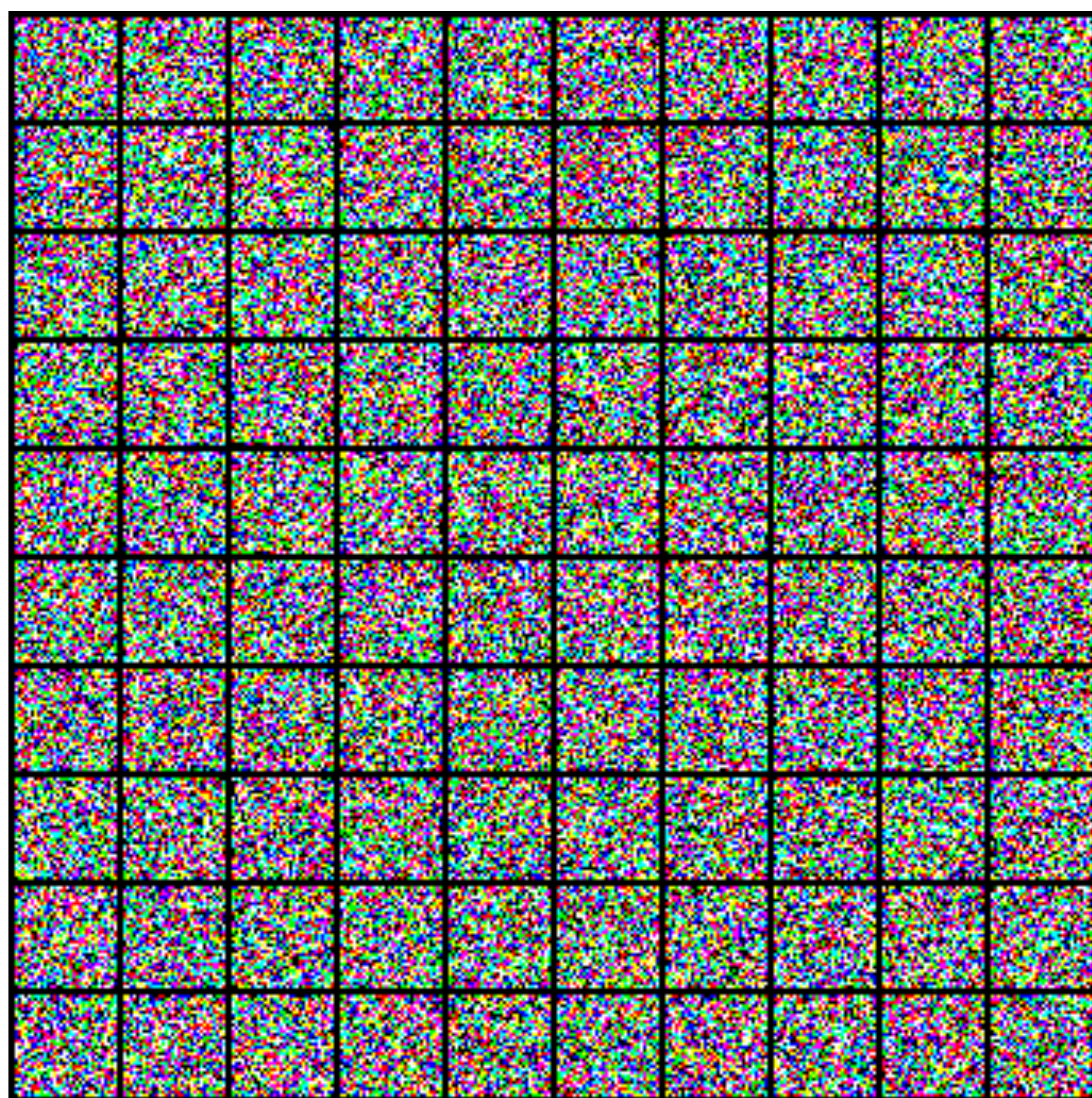
Demo (PFGM word)



Demo (IAFI word)



Experiments: Visualization of Backward ODE



Experiments: Generation Quality and Speed (CIFAR-10)

Model	Invertible?	Quality		Speed
		Inception Score (higher is better)	FID Score (lower is better)	NFE (lower is better)
StyleGAN2-ADA	✗	9.83	2.92	1
Diffusion (VP) - SDE	✗	9.68	2.41	1000
Glow	✓	3.92	48.9	1
Diffusion (VP) - ODE	✓	9.47	2.86	134
PFGM (ours)*	✓	9.68	2.35	110

Current SOTA results in normalizing flow family!

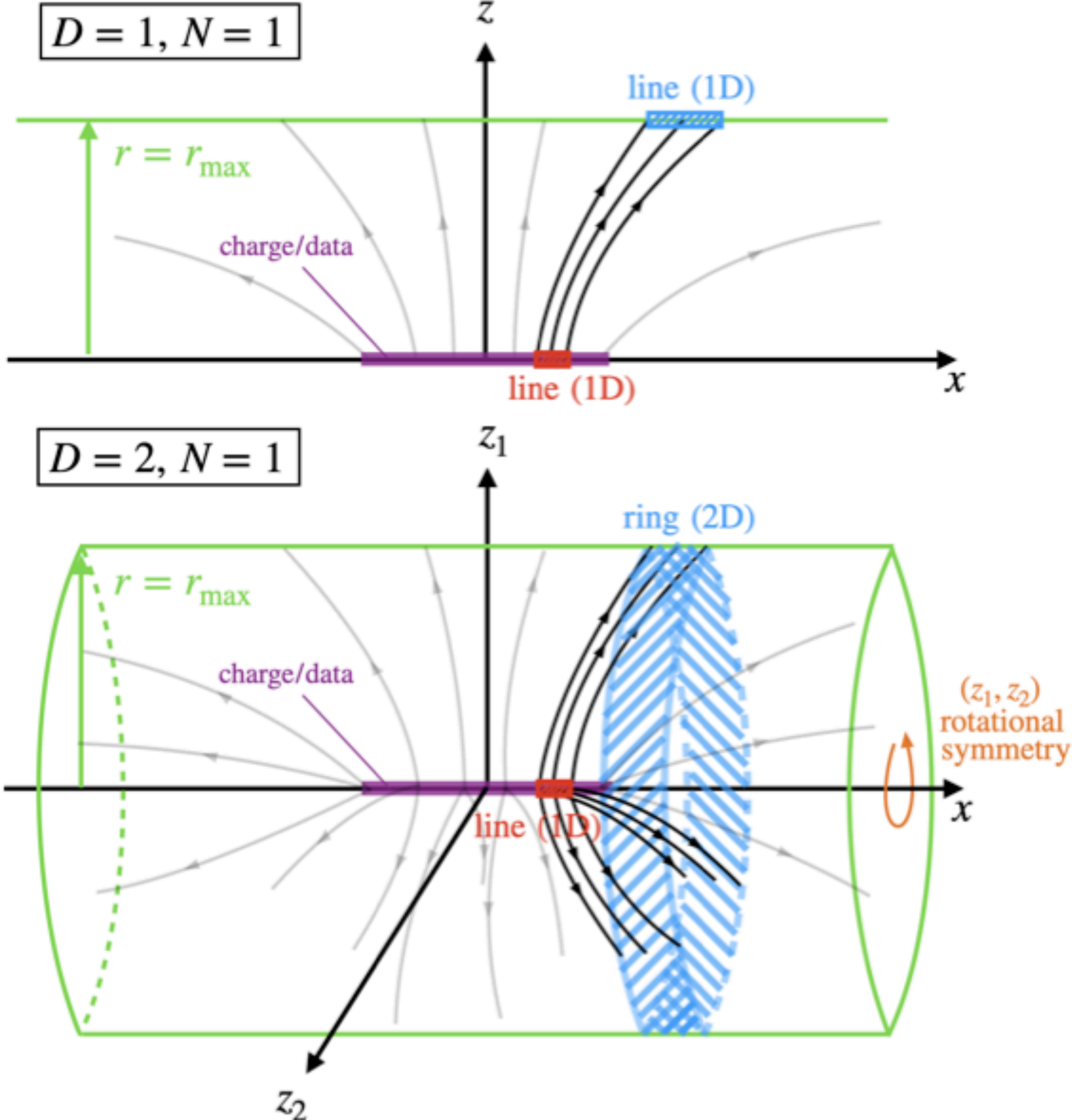
*: PFGM and Diffusion models use the same architecture, DDPM++ deep

**Q: Relation between Diffusion Models and
Poisson Flows?**

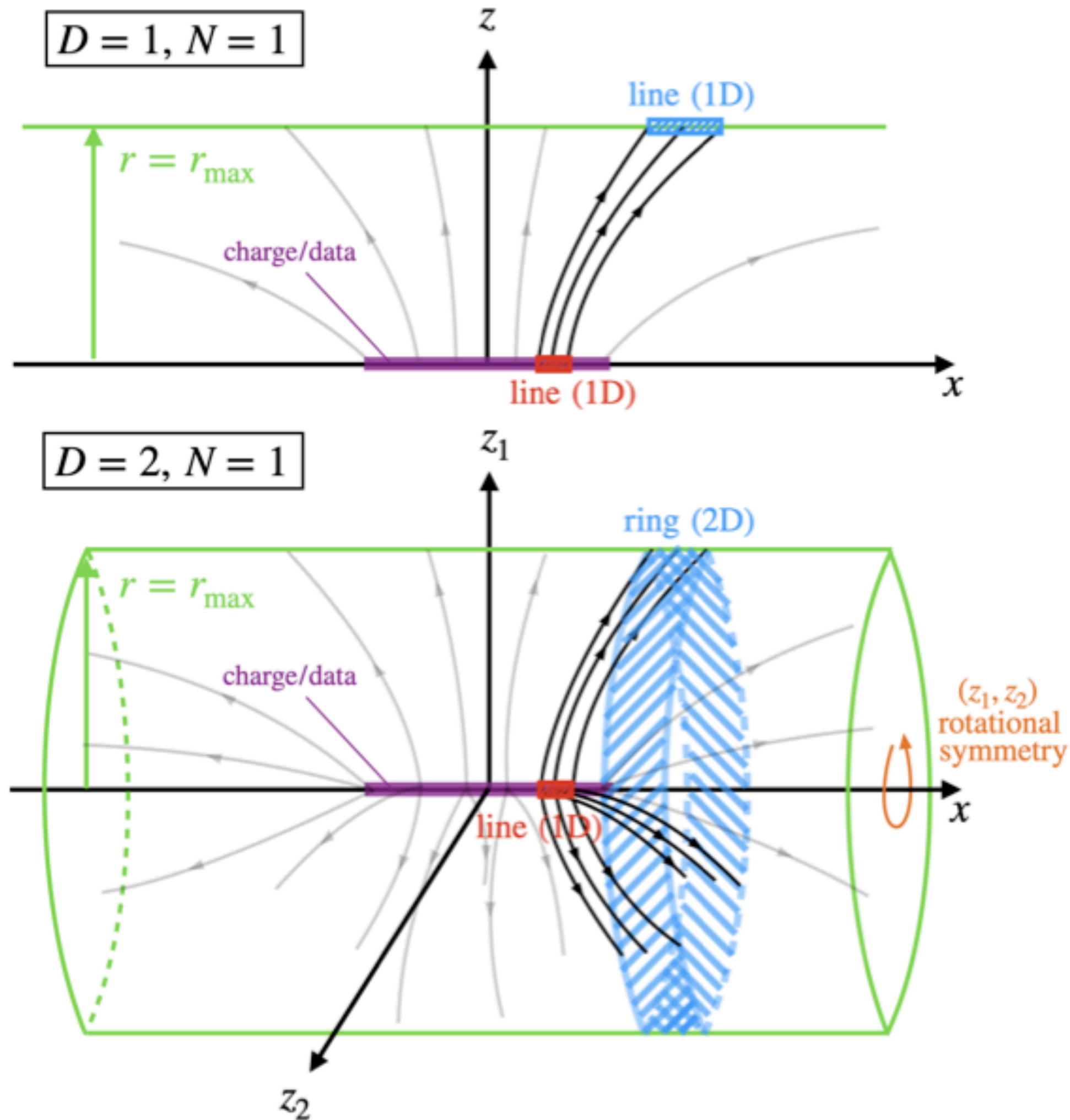
Poisson Flow Generative Models ++

 State of the Art Image Generation on CIFAR-10

Augmented dimensionality D



Anchor the ODE by $r = ||\mathbf{z}||$ due to symmetry



$$\mathbf{E}(\tilde{\mathbf{x}}) = \frac{1}{S_{N+D-1}(1)} \int \frac{\tilde{\mathbf{x}} - \tilde{\mathbf{y}}}{\|\tilde{\mathbf{x}} - \tilde{\mathbf{y}}\|^{N+D}} p(\mathbf{y}) d\mathbf{y}$$

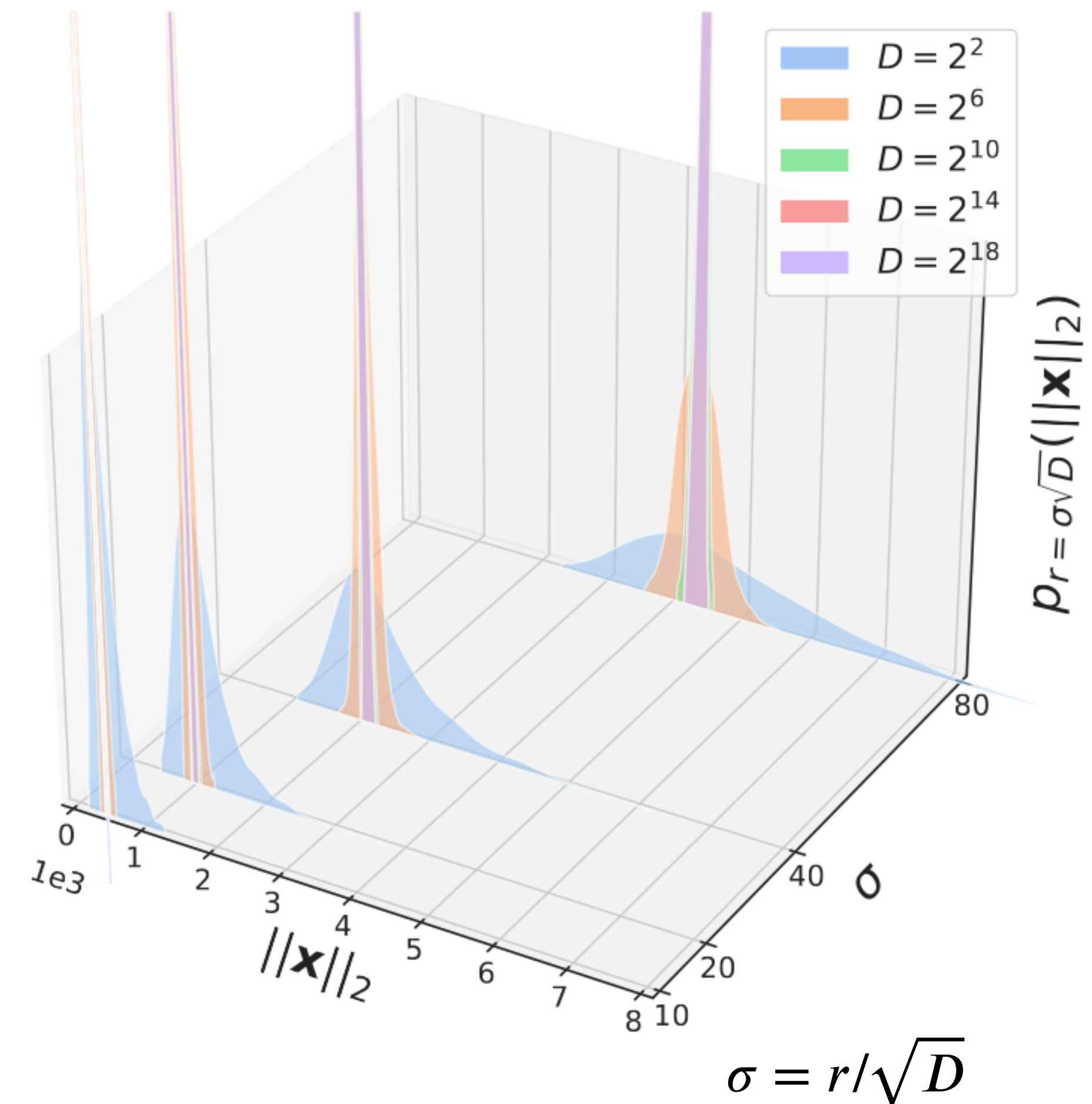
$$d\tilde{\mathbf{x}} = \mathbf{E}(\tilde{\mathbf{x}}) dt$$

$$dz_i = \mathbf{E}(\tilde{\mathbf{x}})_{z_i} dt$$

$$\begin{aligned} \frac{dr}{dt} &= \sum_{i=1}^D \frac{z_i}{r} \frac{dz_i}{dt} = \int \frac{\sum_{i=1}^D z_i^2}{S_{N+D-1}(1)r \|\tilde{\mathbf{x}} - \tilde{\mathbf{y}}\|^{N+D}} p(\mathbf{y}) d\mathbf{y} \\ &= \frac{1}{S_{N+D-1}(1)} \int \frac{r}{\|\tilde{\mathbf{x}} - \tilde{\mathbf{y}}\|^{N+D}} p(\mathbf{y}) d\mathbf{y} \end{aligned}$$

Balance Robustness and Rigidity by Controlling D

- Larger $D \rightarrow$ Better Accuracy/ Worse Robustness
- Smaller $D \rightarrow$ Worse Accuracy/ Better Robustness



Sweet spot D^ in the middle!*

Experiments: Image Generation

Table 1. CIFAR-10 sample quality (FID) and number of function evaluations (NFE).

	Min FID ↓	Top-3 Avg FID ↓	NFE ↓
DDPM (Ho et al., 2020)	3.17	-	1000
DDIM (Song et al., 2021a)	4.67	-	50
VE-ODE (Song et al., 2021b)	5.29	-	194
VP-ODE (Song et al., 2021b)	2.86	-	134
PFGM (Xu et al., 2022)	2.48	-	104
<i>PFGM++ (unconditional)</i>			
$D = 64$	1.96	1.98	35
$D = 128$	1.92	1.94	35
$D = 2048$	1.91	1.93	35
$D = 3072000$	1.99	2.02	35
$D \rightarrow \infty$ (Karras et al., 2022)	1.98	2.00	35
<i>PFGM++ (class-conditional)</i>			
$D = 2048$	1.74	-	35
$D \rightarrow \infty$ (Karras et al., 2022)	1.79	-	35

Table 2. FFHQ sample quality (FID) with 79 NFE in unconditional setting

	Min FID ↓	Top-3 Avg FID ↓
$D = 128$	2.43	2.48
$D = 2048$	2.46	2.47
$D = 3072000$	2.49	2.52
$D \rightarrow \infty$ (Karras et al., 2022)	2.53	2.54

(with improved DDPM++/NCSN++ backbone in EDM)

Experiments: Image Generation

Table 1. CIFAR-10 sample quality (FID) and number of function evaluations (NFE).

	Min FID ↓	Top-3 Avg FID ↓	NFE ↓
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$D = 2048$	1.74	-	35
$D \rightarrow \infty$ (Karras et al., 2022)	1.79	-	35

State of the Art Image Generation on CIFAR-10

Filter: GAN Score-based VAE Flow-based Transformer Diffusion PFGM ResNet Optimal Transport EBM [Edit Leaderboard](#)

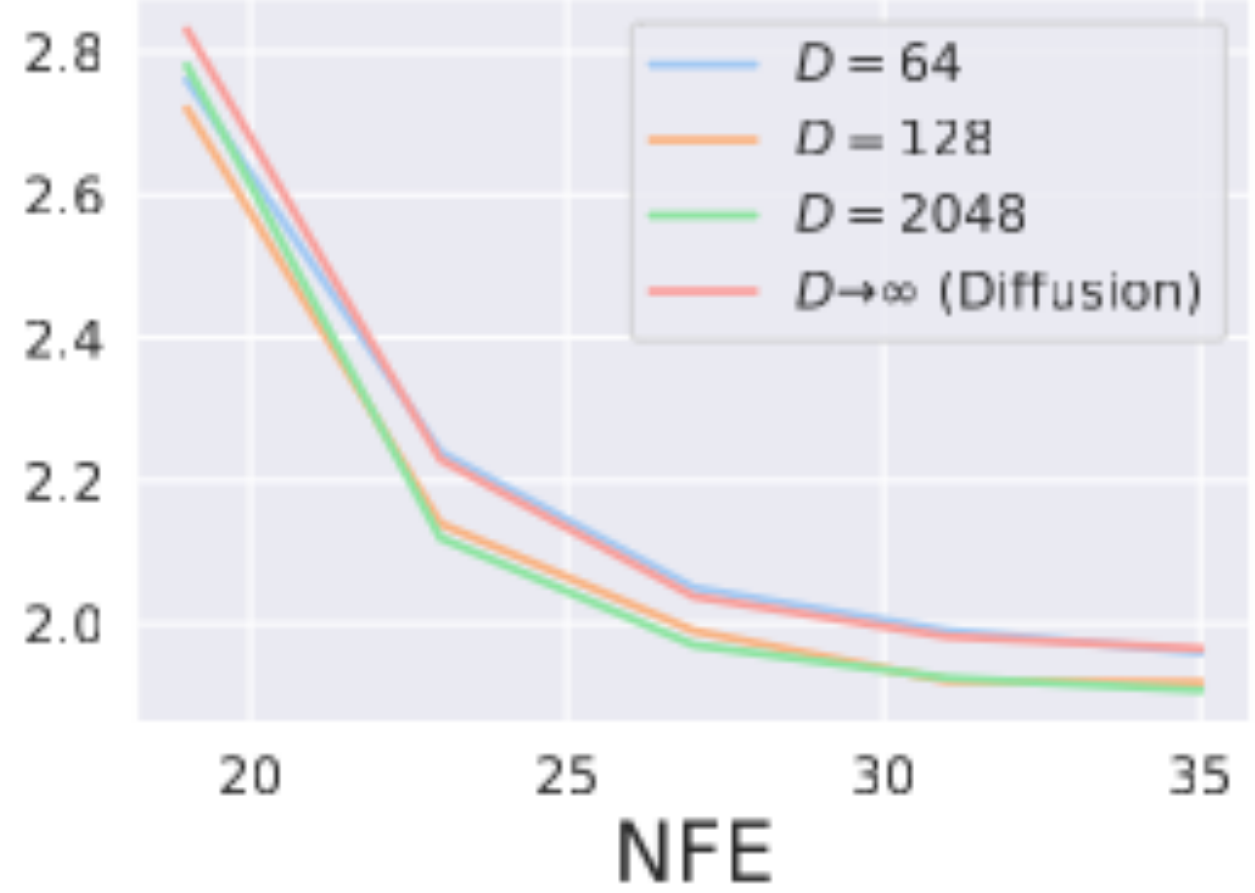
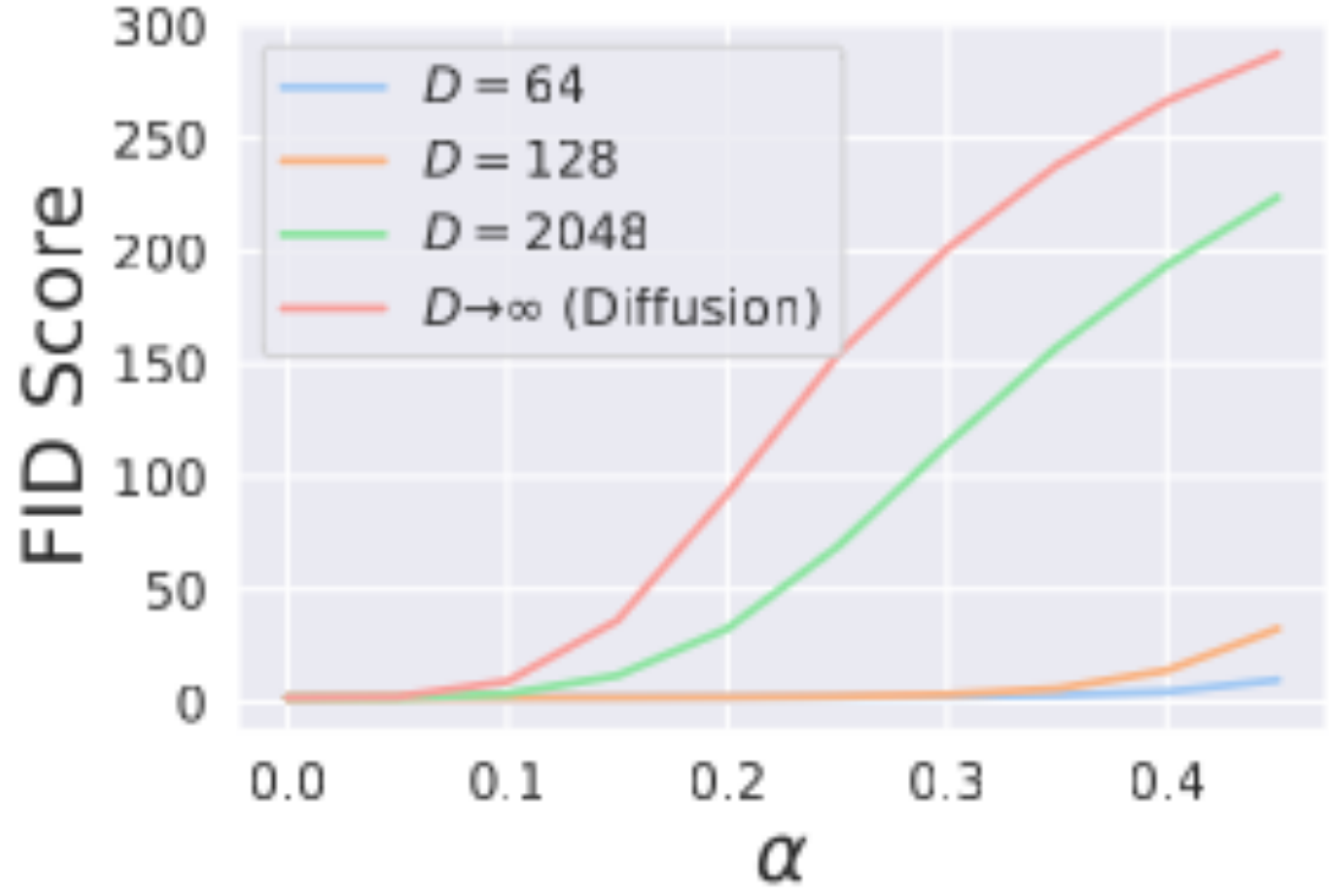
untagged

Rank	Model	Clean-FID ↓	FID-10k	Inception score	bits/dimension	FID-10k-test	Paper	Code	Result	Year	Tags
1	PFGM++	1.74					PFGM++: Unlocking the Potential of Physics-Inspired Generative Models	Code	Result	2023	PFGM
2	EDM-G++ (unconditional)	1.77			2.55		Refining Generative Process with Discriminator Guidance in Score-based Diffusion Models	Code	Result	2022	Diffusion Score-based
3	StyleGAN-XL	1.85					StyleGAN-XL: Scaling StyleGAN to Large Diverse Datasets	Code	Result	2022	GAN
4	STF (unconditional)	1.90					Stable Target Field for Reduced Variance Score Estimation in Diffusion Models	Code	Result	2023	Score-based
5	LSGM-G++ (FID)	1.94			3.42		Refining Generative Process with Discriminator Guidance in Score-based Diffusion Models	Code	Result	2022	Score-based
6	LSGM (FID)	2.10			3.43		Score-based Generative Modeling in Latent Space	Code	Result	2021	Score-based VAE
7	Subspace Diffusion (NSCN++)	2.17		9.99			Subspace Diffusion Generative Models	Code	Result	2022	Score-based
8	LSGM (balanced)	2.17			2.95		Score-based Generative Modeling in Latent Space	Code	Result	2021	VAE Score-based
9	NCSN++	2.20		9.73			Score-Based Generative Modeling through Stochastic Differential Equations	Code	Result	2020	Score-based

<https://paperswithcode.com/sota/image-generation-on-cifar-10>

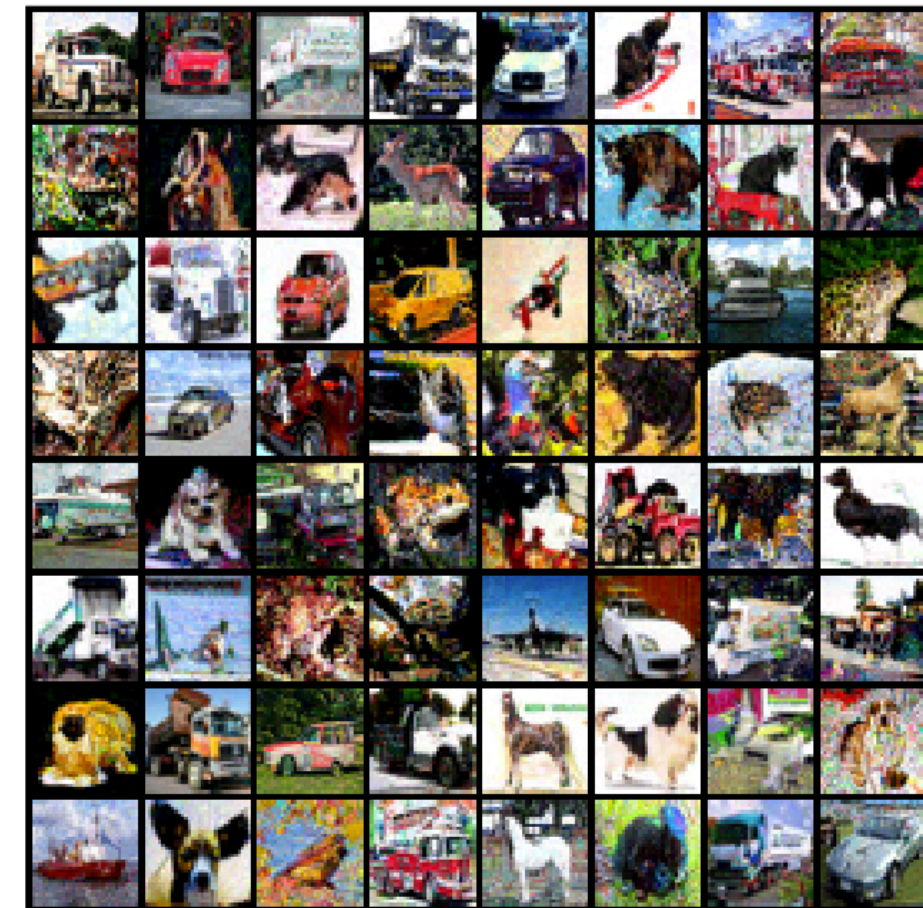
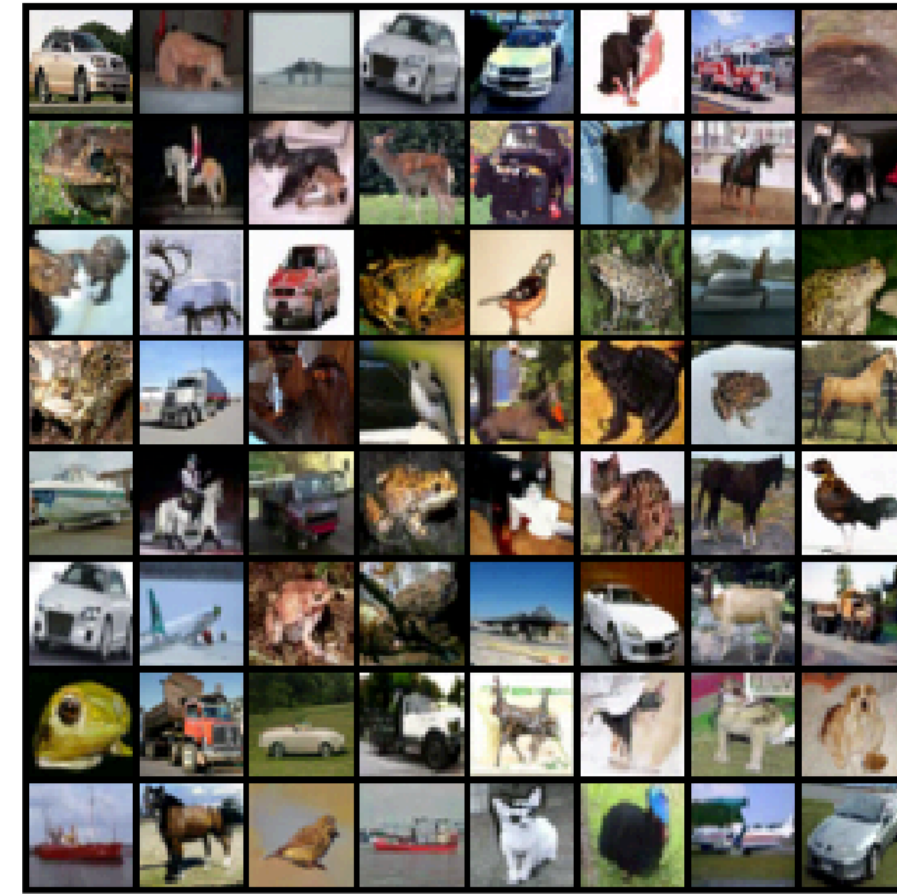
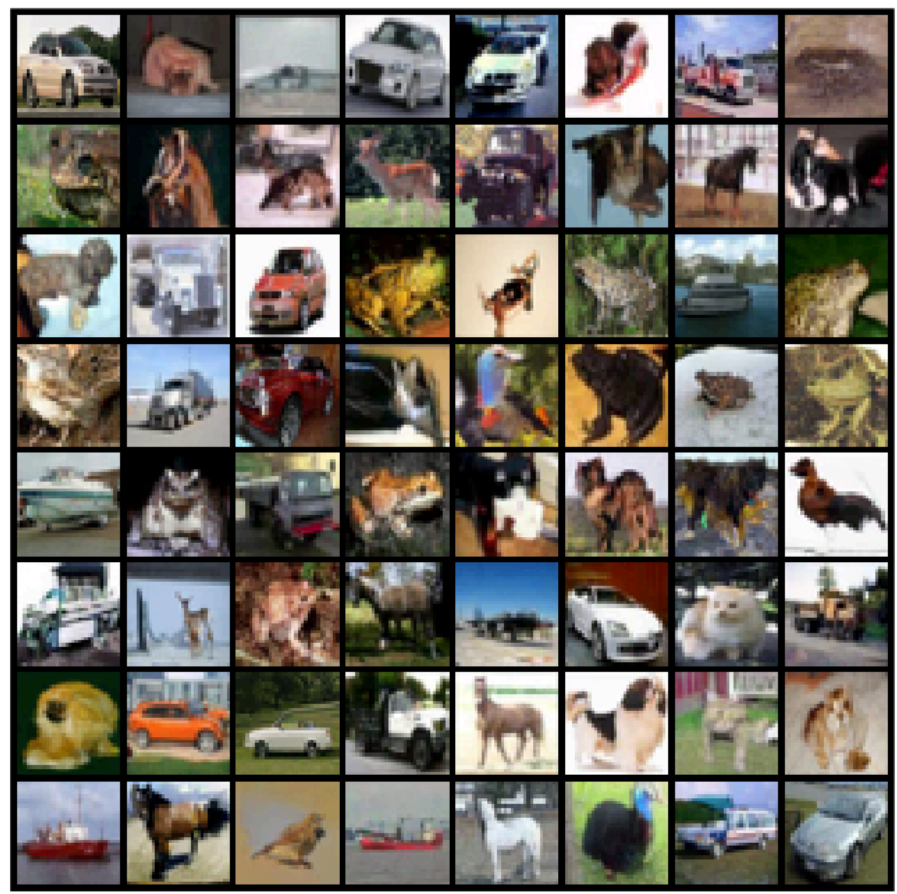
Experiments: Robustness

α : noise scale



$D =$ **64** **128** **2048** ∞

$\alpha = 0.2$



Experiments: Robustness in post-training quantization

Table 3. FID score versus quantization bit-widths on CIFAR-10.

<i>Quantization bits:</i>	9	8	7	6	5
$D = 64$	1.96	1.96	2.12	2.94	28.50
$D = 128$	1.93	1.97	2.15	3.68	34.26
$D = 2048$	1.91	1.97	2.12	5.67	47.02
$D \rightarrow \infty$	1.97	2.04	2.16	5.91	50.09

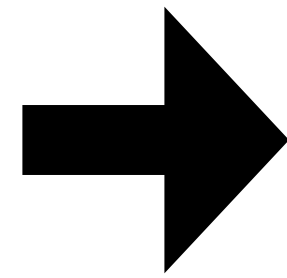
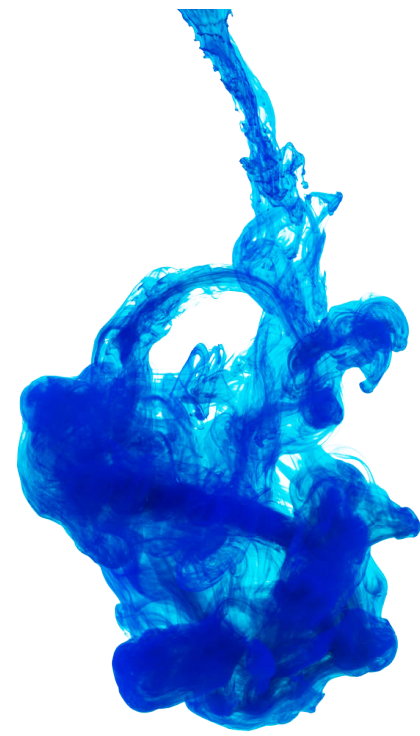
**Q: Going beyond diffusion equation and
Poisson equation?**

GenPhys: From Physical Processes to Generative Models

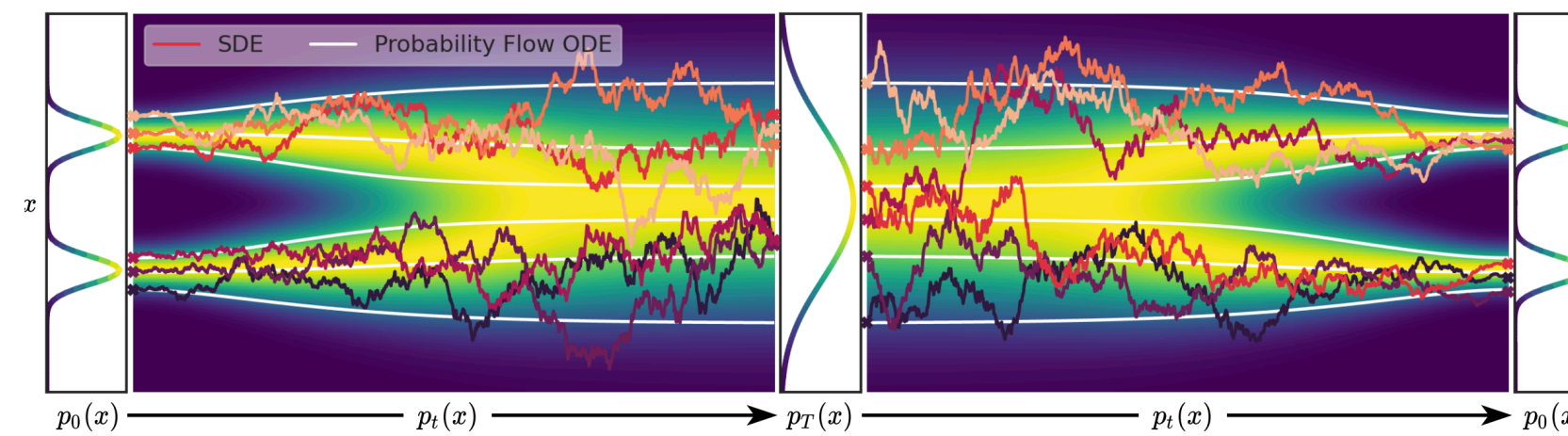
Ziming Liu, Di Luo, Yilun Xu, Tommi Jaakkola, Max Tegmark. “GenPhys: From Physical Processes to Generative Models”
arXiv: 2304.02637

From physics to generative models

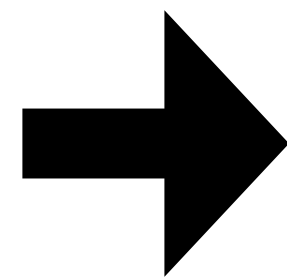
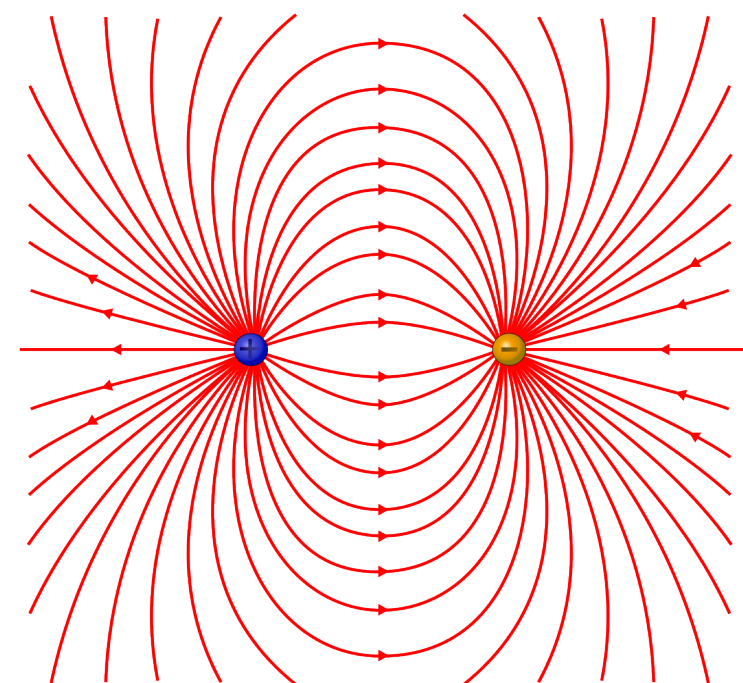
Diffusion
(Diffusion equation)



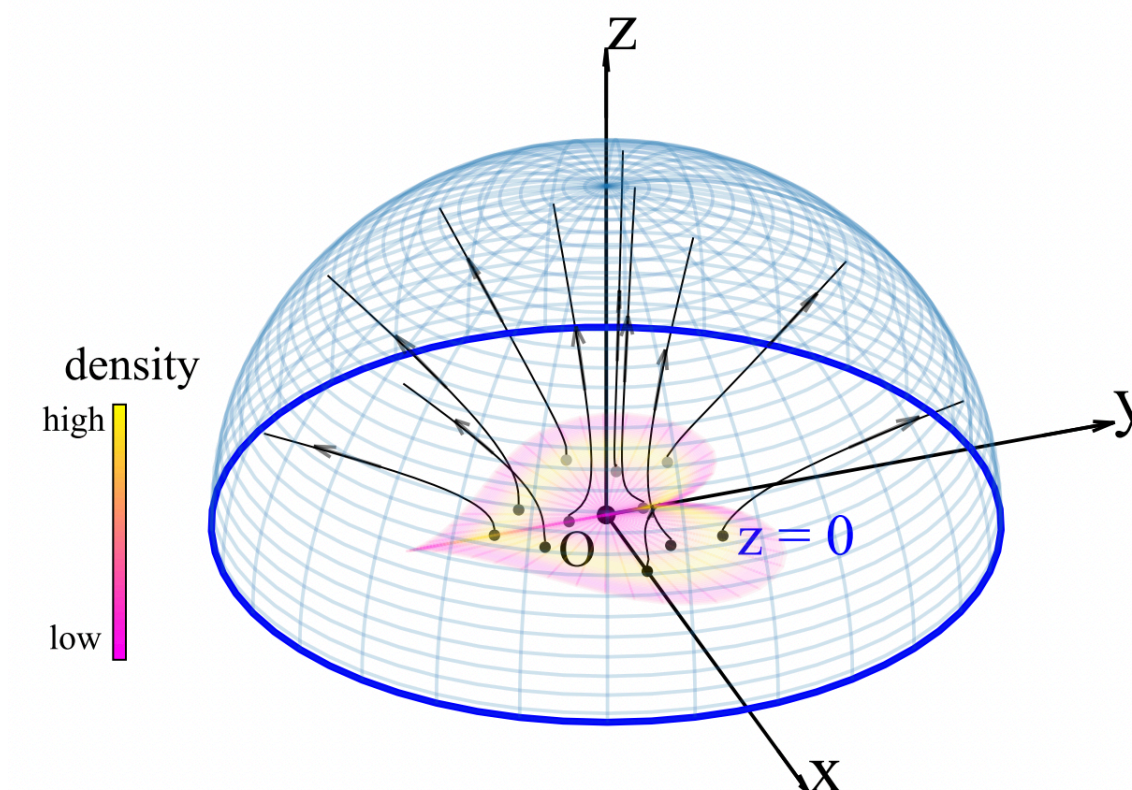
Diffusion models



Electrostatics
(Poisson equation)



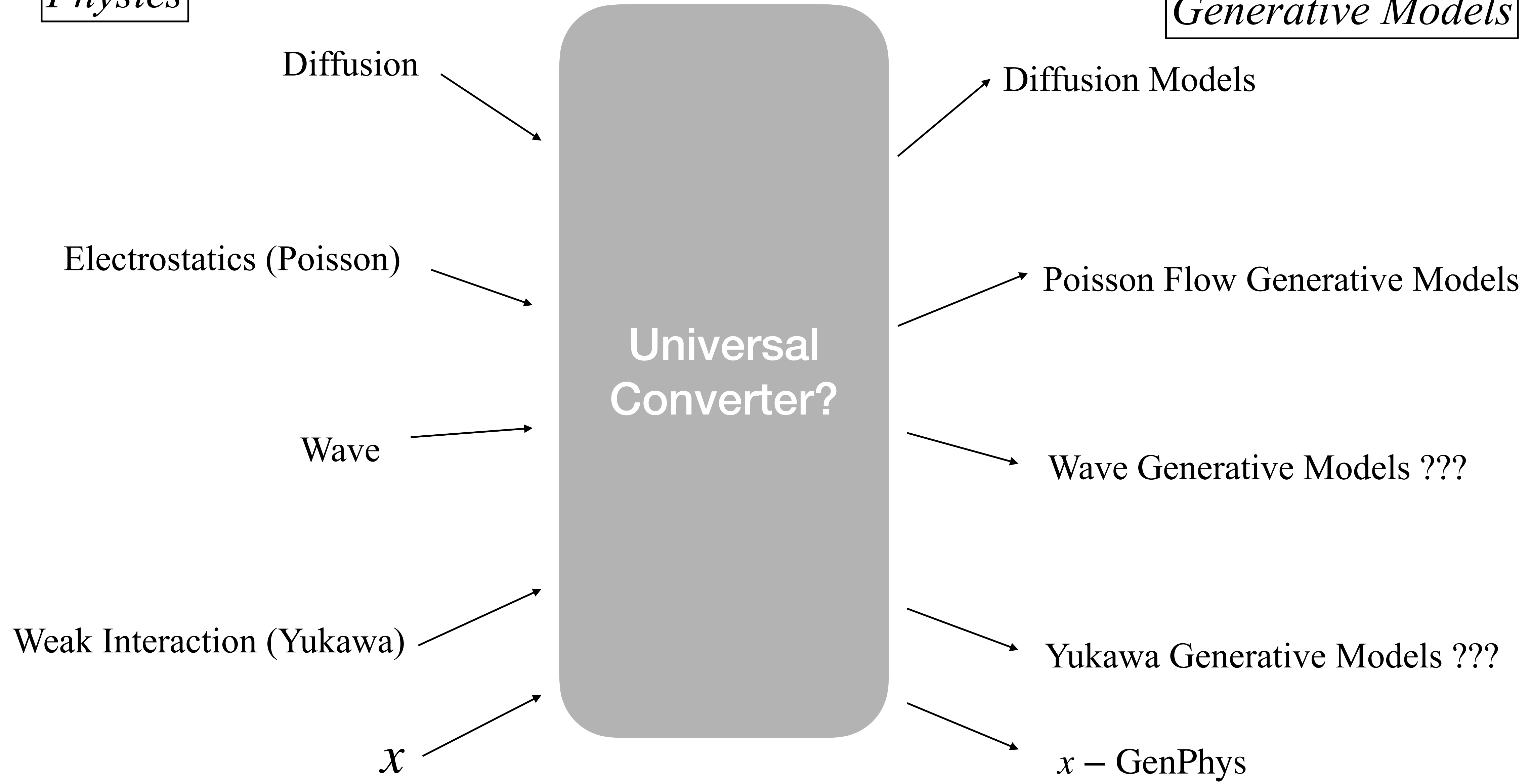
Poisson Flow Generative Models



From physics to generative models?

Physics

Generative Models

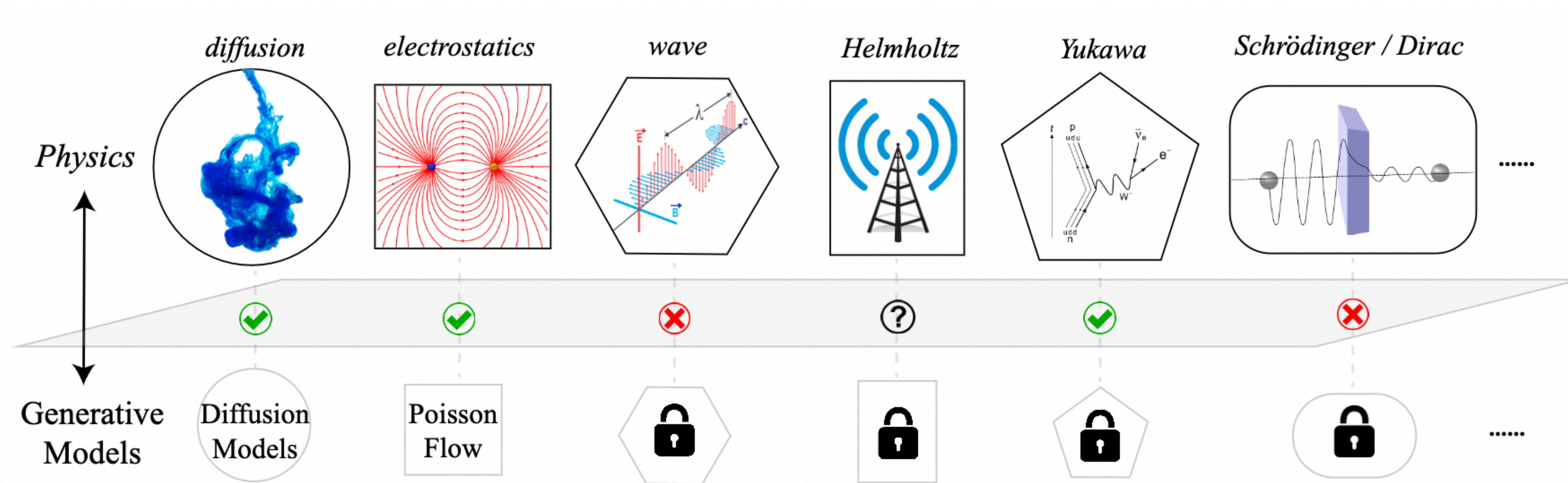


Q: Is there a universal converter from physics to generative models?

A: **Yes, but...**

Yes: A concrete protocol that converts physics to generative models

but: the converted generative models may not have desirable properties



Converter: partial differential equations (PDEs)

A *physical process* is described by a **PDE**

$$\hat{L}\phi \equiv F(\phi, \phi_t, \phi_{tt}, \nabla\phi, \nabla^2\phi, \dots) = f(\mathbf{x}, t) \quad (\text{Physical PDE})$$

Physicists already know how to solve it, ...

..., if they are equivalent, ...

A *generative model* is associated with a density flow (which is also a **PDE**)

$$\hat{M}(p, \mathbf{v}, R) \equiv \frac{\partial p(\mathbf{x}, t)}{\partial t} + \nabla \cdot [p(\mathbf{x}, t)\mathbf{v}(\mathbf{x}, t)] - R(\mathbf{x}, t) = p_{\text{data}}(\mathbf{x})\delta(t) \quad (\text{Density Flow})$$

probability distribution velocity field birth/death rate

..., then we know how to solve this one, too. By “solve”, we mean a design of (p, \mathbf{v}, R) .

Converter

physical process

$$\hat{L}\phi \equiv F(\phi, \phi_t, \phi_{tt}, \nabla\phi, \nabla^2\phi, \dots) = f(\mathbf{x}, t) \quad (\text{Physical PDE})$$

generative model

$$\hat{M}(p, \mathbf{v}, R) \equiv \frac{\partial p(\mathbf{x}, t)}{\partial t} + \nabla \cdot [p(\mathbf{x}, t)\mathbf{v}(\mathbf{x}, t)] - R(\mathbf{x}, t) = p_{\text{data}}(\mathbf{x})\delta(t) \quad (\text{Density Flow})$$

???

Simply set $f(\mathbf{x}, t) = p_{\text{data}}(\mathbf{x})\delta(t)$

Example: Diffusion equation

Source PDE

$$\phi_t - \nabla^2 \phi = 0$$

Target PDE

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} + \nabla \cdot [p(\mathbf{x}, t)\mathbf{v}(\mathbf{x}, t)] - R(\mathbf{x}, t) = 0$$

$$\phi_t - \nabla^2 \phi = \frac{\partial \phi}{\partial t} + \nabla \cdot (\phi(-\nabla \log \phi)) - 0 \quad \Leftrightarrow \quad \frac{\partial p}{\partial t} + \nabla \cdot (p\mathbf{v}) - R$$

Comparing the two sides gives:

$$p = \phi, \quad \underline{\mathbf{v} = -\nabla \log \phi}, \quad R = 0$$

“score”

Example: Poisson equation

Source PDE

$$\phi_{tt} + \nabla^2 \phi = 0$$

Target PDE

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} + \nabla \cdot [p(\mathbf{x}, t)\mathbf{v}(\mathbf{x}, t)] - R(\mathbf{x}, t) = 0$$

$$-(\phi_{tt} + \nabla^2 \phi) = \frac{(\partial - \phi_t)}{\partial t} + \nabla \cdot \left[-\phi_t \left(\frac{\nabla \phi}{\phi_t} \right) \right] - 0 \Leftrightarrow \frac{\partial p}{\partial t} + \nabla \cdot (p\mathbf{v}) - R$$

Comparing the two sides gives:

$$p = -\phi_t, \quad \mathbf{v} = \frac{\nabla \phi}{\phi_t}, \quad R = 0$$

“Poisson field”

Example: Wave equation

Source PDE

$$\phi_{tt} - \nabla^2 \phi = 0$$

Target PDE

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} + \nabla \cdot [p(\mathbf{x}, t)\mathbf{v}(\mathbf{x}, t)] - R(\mathbf{x}, t) = 0$$

$$-(\phi_{tt} - \nabla^2 \phi) = \frac{(\partial - \phi_t)}{\partial t} + \nabla \cdot \left[-\phi_t \left(-\frac{\nabla \phi}{\phi_t} \right) \right] - 0 \Leftrightarrow \frac{\partial p}{\partial t} + \nabla \cdot (p\mathbf{v}) - R$$

Comparing the two sides gives:

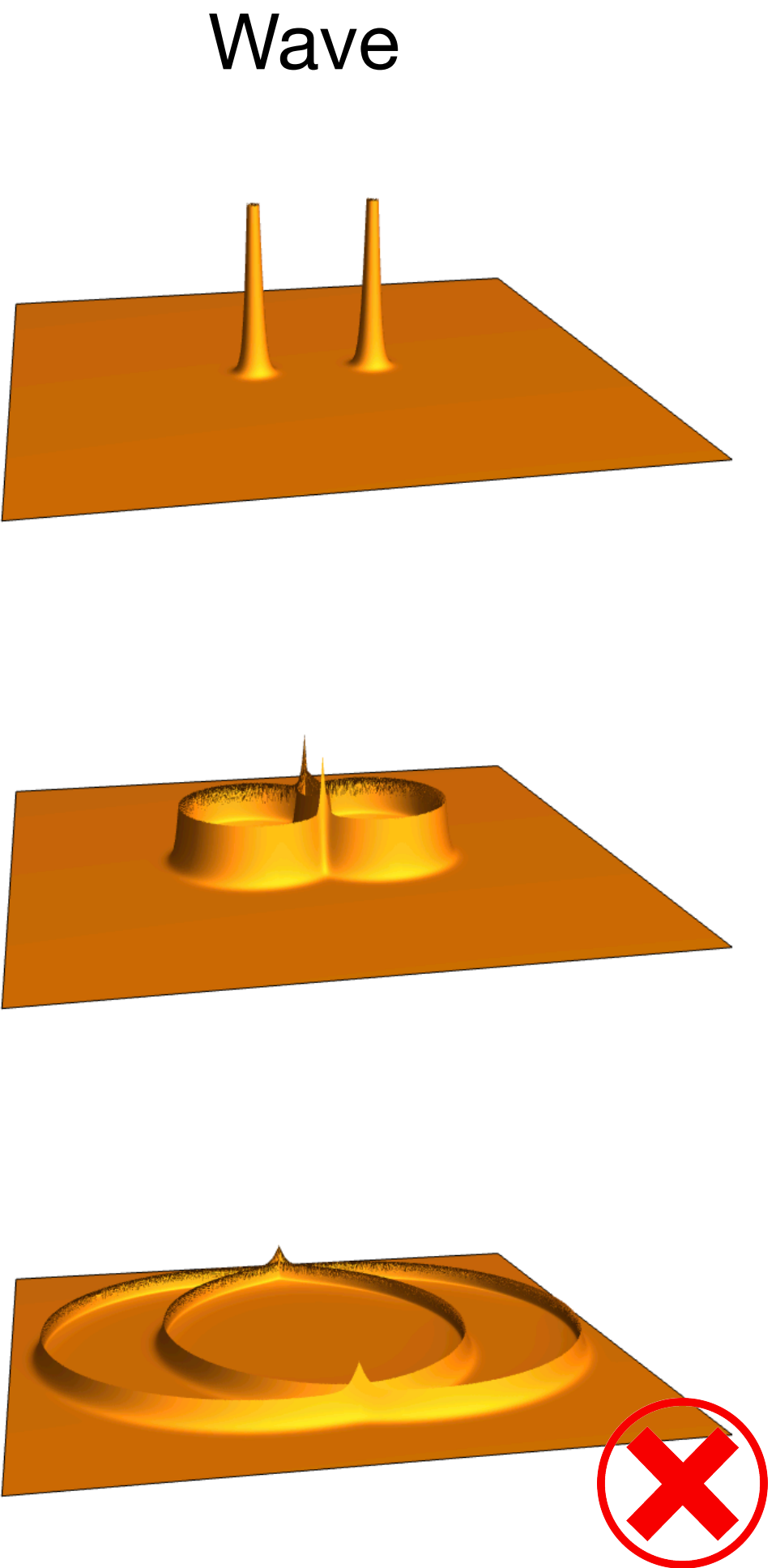
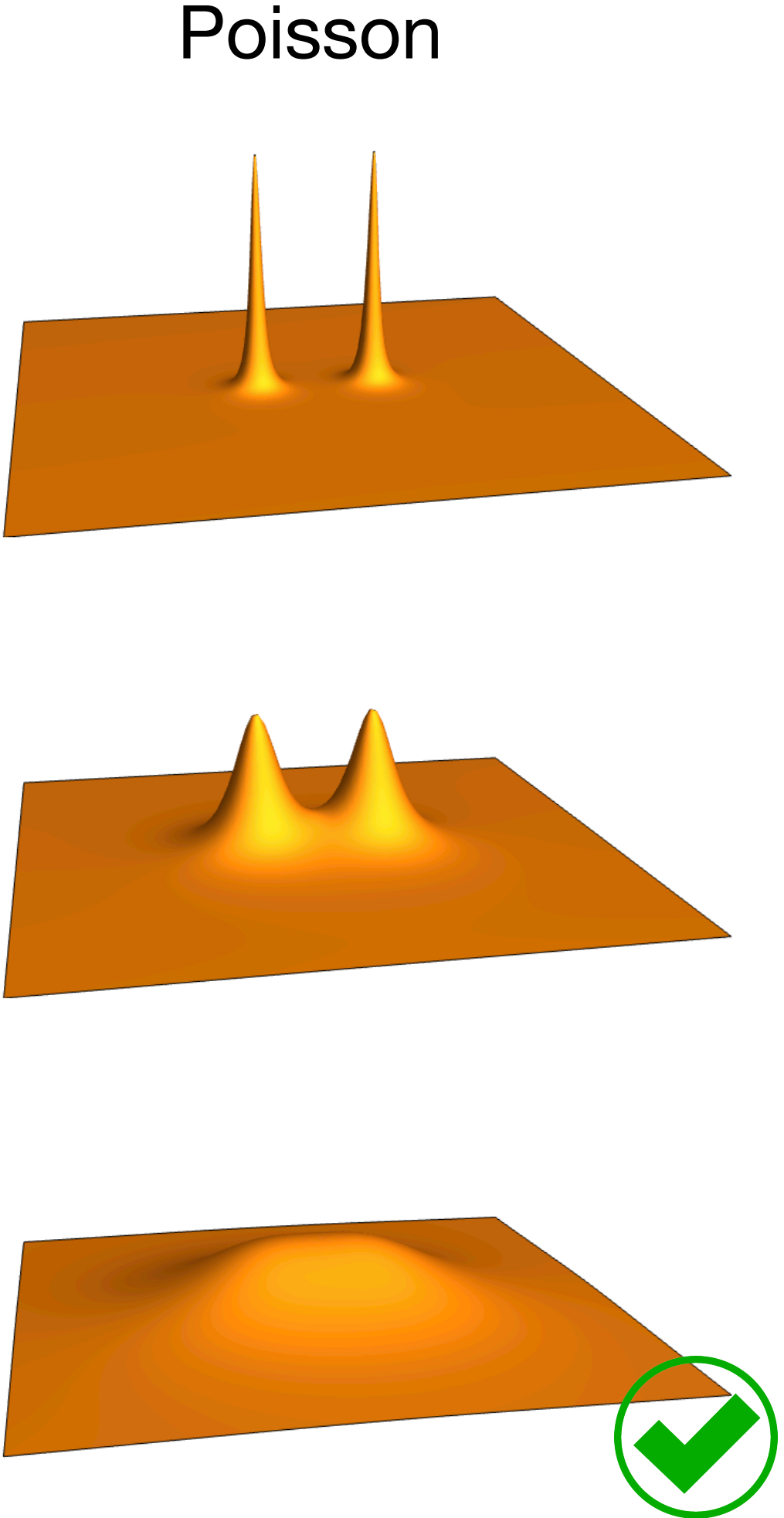
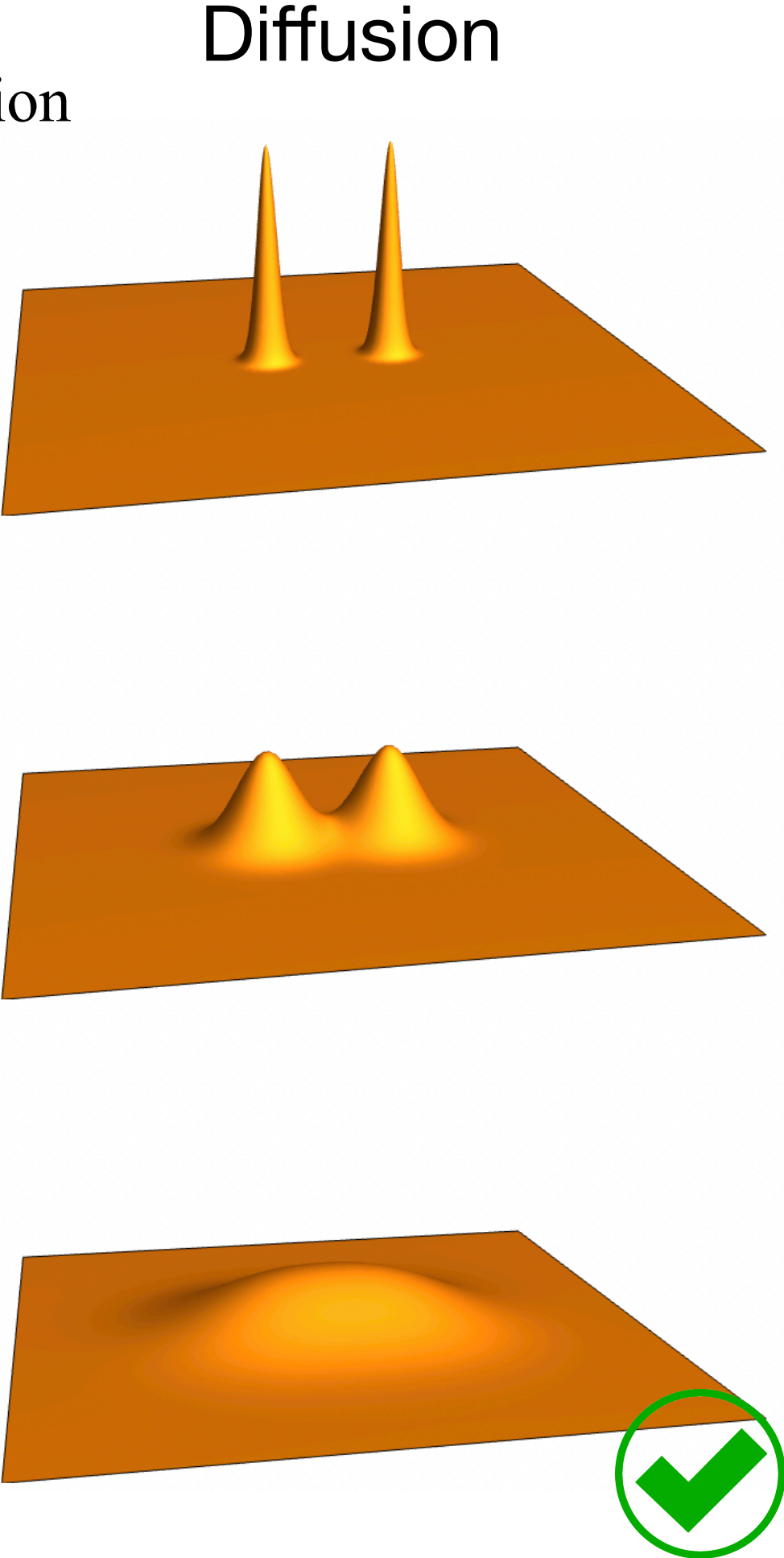
$$p = -\phi_t, \quad \mathbf{v} = -\frac{\nabla \phi}{\phi_t}, \quad R = 0$$

BUT WAIT!

Caveat: prior distribution

Generative models should have data-independent priors:
No matter what the initial distribution (data) is, the final distribution should be independent of it.

Toy:
Two point distribution



Time



Which PDEs can give desirable generative models?

A PDE x is *s-generative* (s for smooth) if:

(C1) x can be converted to a density flow;

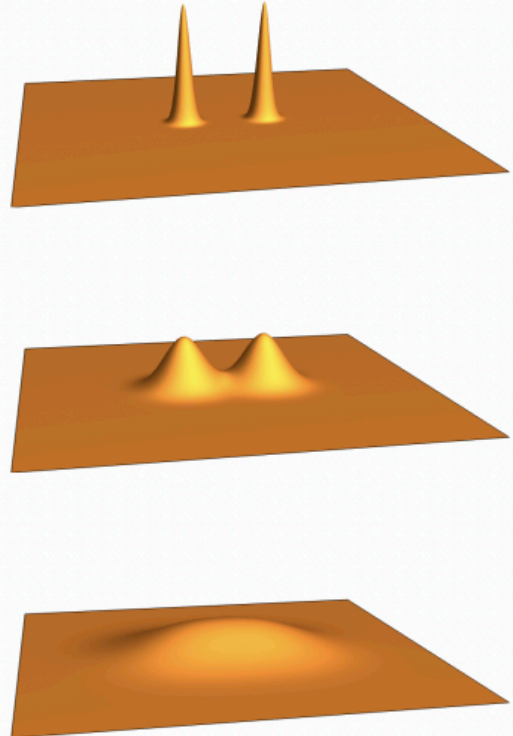
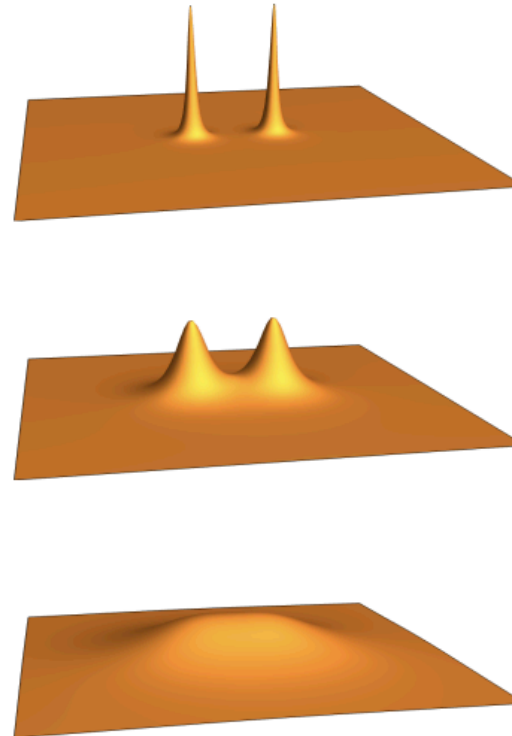
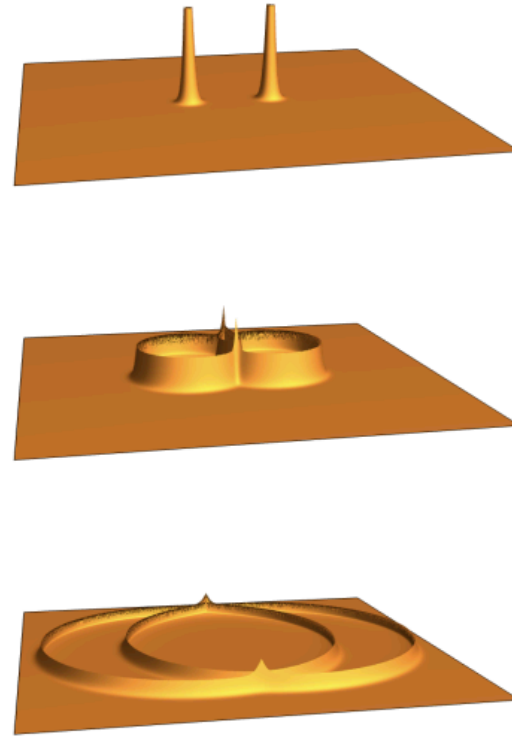
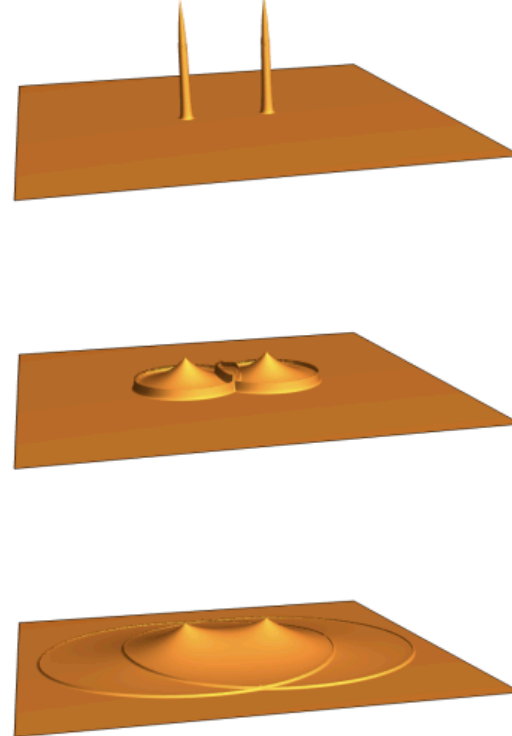
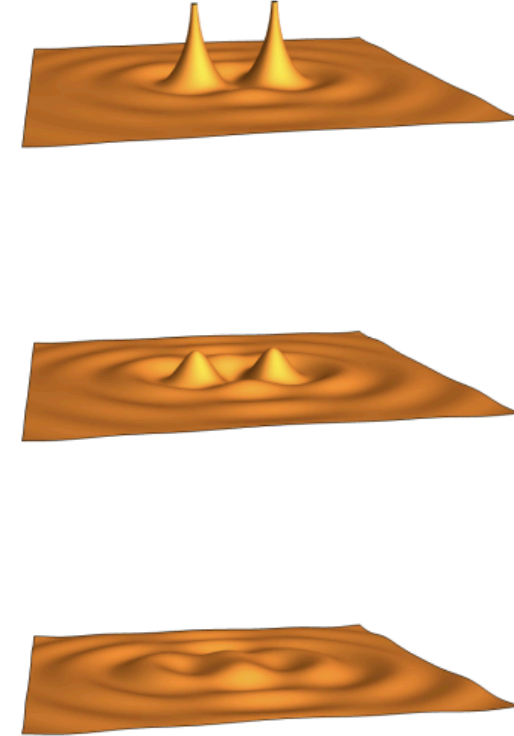
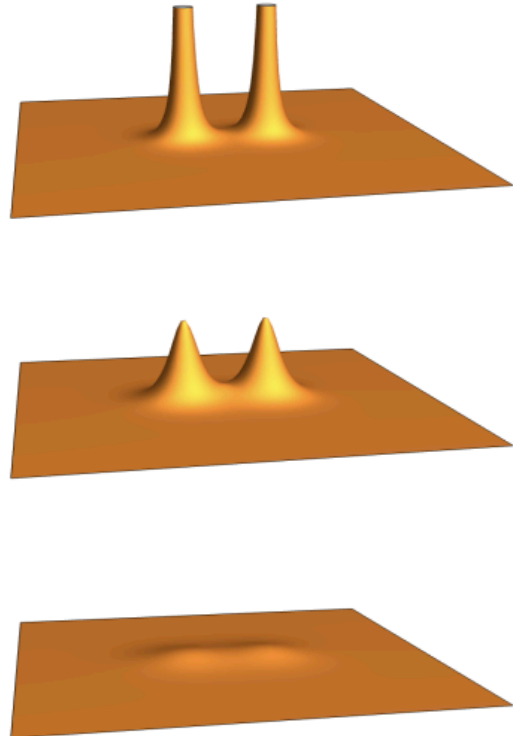
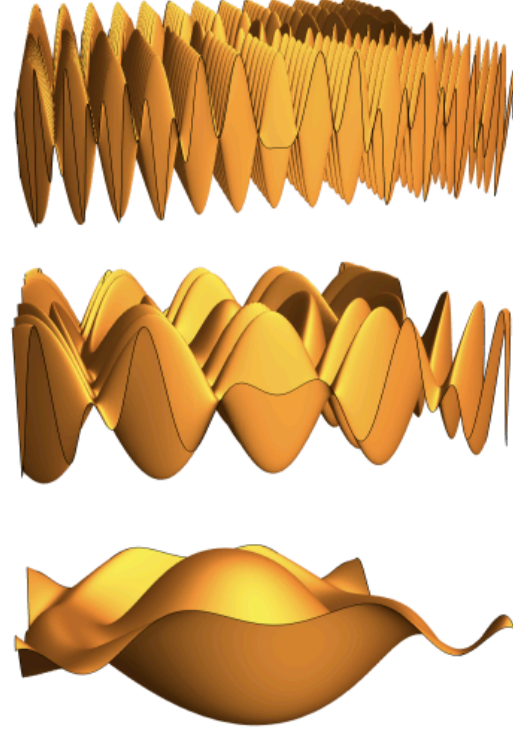
(C2) The solutions of x become “smoother” over time.

(C1) Case-dependent constructions are required, but are usually straightforward.

(C2) turns out to be equivalent to a constraint on dispersion relations of PDEs.

Intuition: Non-zero frequency modes should decay faster than zero modes.

Examples

	✔	✔	✘	?	?	✔	✘
equation	diffusion equation	Poisson equation	ideal wave equation	dissipative wave equation	Helmholtz equation	screened Poisson equation (Yukawa)	Schrödinger equation
PDE $\hat{L}\phi = 0$	$\phi_t - \nabla^2\phi = 0$	$\phi_{tt} + \nabla^2\phi = 0$	$\phi_{tt} - \nabla^2\phi = 0$	$\phi_{tt} + 2\epsilon\phi_t - \nabla^2\phi = 0$	$\phi_{tt} + \nabla^2\phi + k_0^2\phi = 0$	$\phi_{tt} + \nabla^2\phi - m^2\phi = 0$	$i\phi_t + \nabla^2\phi = 0$
Rewritten	$\frac{\partial\phi}{\partial t} + \nabla \cdot (\phi(-\nabla\log\phi)) = 0$	$\frac{\partial(-\phi_t)}{\partial t} + \nabla \cdot ((-\phi_t)(\frac{\nabla\phi}{\phi_t})) = 0$	$\frac{\partial(-\phi_t)}{\partial t} + \nabla \cdot ((-\phi_t)(-\frac{\nabla\phi}{\phi_t})) = 0$	$\frac{\partial(-\phi_t - 2\epsilon\phi)}{\partial t} + \nabla \cdot ((-\phi_t - 2\epsilon\phi)(\frac{\nabla\phi}{\phi_t + 2\epsilon\phi})) = 0$	$\frac{\partial(-\phi_t)}{\partial t} + \nabla \cdot ((-\phi_t)(\frac{\nabla\phi}{\phi_t})) - k_0^2\phi = 0$	$\frac{\partial(-\phi_t)}{\partial t} + \nabla \cdot ((-\phi_t)(\frac{\nabla\phi}{\phi_t})) + m^2\phi = 0$	$\frac{\partial \phi ^2}{\partial t} + \nabla \cdot (\phi ^2(2\text{Im}\nabla\log\phi)) = 0$
p	ϕ	$-\phi_t$	$-\phi_t$	$-(\phi_t + 2\epsilon\phi)$	$-\phi_t$	$-\phi_t$	$ \phi ^2$
\mathbf{v}	$-\nabla\log\phi$	$\frac{\nabla\phi}{\phi_t}$	$-\frac{\nabla\phi}{\phi_t}$	$\frac{\nabla\phi}{\phi_t + 2\epsilon\phi}$	$-\phi_t$	$-\phi_t$	$ \phi ^2$
R	0	0	0	0	$k_0^2\phi$	$-m^2\phi$	0
$G(r, t)$	$\frac{1}{(4\pi t)^{\frac{N}{2}}} \exp(-\frac{r^2}{4t})$	$\frac{1}{(t^2+r^2)^{\frac{N-1}{2}}}$	$\frac{1}{\sqrt{t^2-r^2}} \Theta(t-r)$ (2D)	$\frac{e^{-\epsilon t} \cosh(\epsilon\sqrt{t^2-r^2})}{\sqrt{t^2-r^2}} \Theta(t-r)$ (2D)	$(\frac{k_0}{\sqrt{t^2+r^2}})^{\frac{N-1}{2}} H_{\frac{N-1}{2}}^{(1)}(k_0\sqrt{t^2+r^2})$	$(\frac{m}{\sqrt{t^2+r^2}})^{\frac{N-1}{2}} K_{\frac{N-1}{2}}(m\sqrt{t^2+r^2})$	$\frac{1}{(4\pi it)^{\frac{N}{2}}} \exp(\frac{ir^2}{4t})$
$\hat{G}(k, t)$	$\exp(-k^2t)$	$\exp(-kt)$	$\exp(\pm ikt)$	$\exp(-\epsilon t + i\sqrt{k^2 - \epsilon^2}t)$ ($k > \epsilon$) $\exp(-(\epsilon + \sqrt{k^2 - \epsilon^2})t)$ ($k \leq \epsilon$) $\hat{G}(k, t)$	$\exp(-i\sqrt{k_0^2 - k^2}t)$ ($k \leq k_0$) $\exp(-\sqrt{k^2 - k_0^2}t)$ ($k > k_0$)	$\exp(-\sqrt{k^2 + m^2}t)$	$\exp(ik^2t)$
(C1)	Yes	Yes	No	Conditionally yes	Conditional yes	Yes	No
(C2)	Yes	Yes	No	Conditionally yes	Conditional Yes	Yes	No
Illustration ϕ							
s-generative?	Yes (Diffusion Models)	Yes (Poisson Flow)	No	Conditionally Yes (large ϵ)	Conditionally yes (small k)	Yes	No

Dispersion relations

(C2) The solutions of x become “smoother” over time.

$$\phi \sim e^{i(kx - \omega t)}$$

Table 3: Dispersion relation $\omega(k)$ of physical PDEs.

Physics	PDE	Dispersion Relation	s-generative?
Diffusion	$\phi_t - \nabla^2 \phi = 0$	$\omega = -ik^2$	Yes
Poisson	$\phi_{tt} + \nabla^2 \phi = 0$	$\omega = \pm ik$	Yes
Ideal Wave	$\phi_{tt} - \nabla^2 \phi = 0$	$\omega = \pm k$	No
Dissipative wave	$\phi_{tt} + 2\epsilon\phi_t - \nabla^2 \phi = 0$	$\omega = \begin{cases} i(-\epsilon \pm \sqrt{\epsilon^2 - k^2}) & k \leq \epsilon \\ i\epsilon \pm \sqrt{k^2 - \epsilon^2} & k > \epsilon \end{cases}$	Conditionally Yes (large ϵ)
Helmholtz	$\phi_{tt} + \nabla^2 \phi + k_0^2 \phi = 0$	$\omega = \begin{cases} \pm \sqrt{k_0^2 - k^2} & k \leq k_0 \\ \pm i\sqrt{k^2 - k_0^2} & k > k_0 \end{cases}$	Conditionally Yes (small k_0^2)
Screened Poisson	$\phi_{tt} + \nabla^2 \phi - m^2 \phi = 0$	$\omega = \pm i\sqrt{k^2 + m^2}$	Yes
Schrödinger	$i\phi_t + \nabla^2 \phi = 0$	$\omega = k^2$	No

Smoothing



$\text{Im } \omega(k) < \text{Im } \omega(0), \quad \text{for all } k > 0$

Other s-generative PDEs

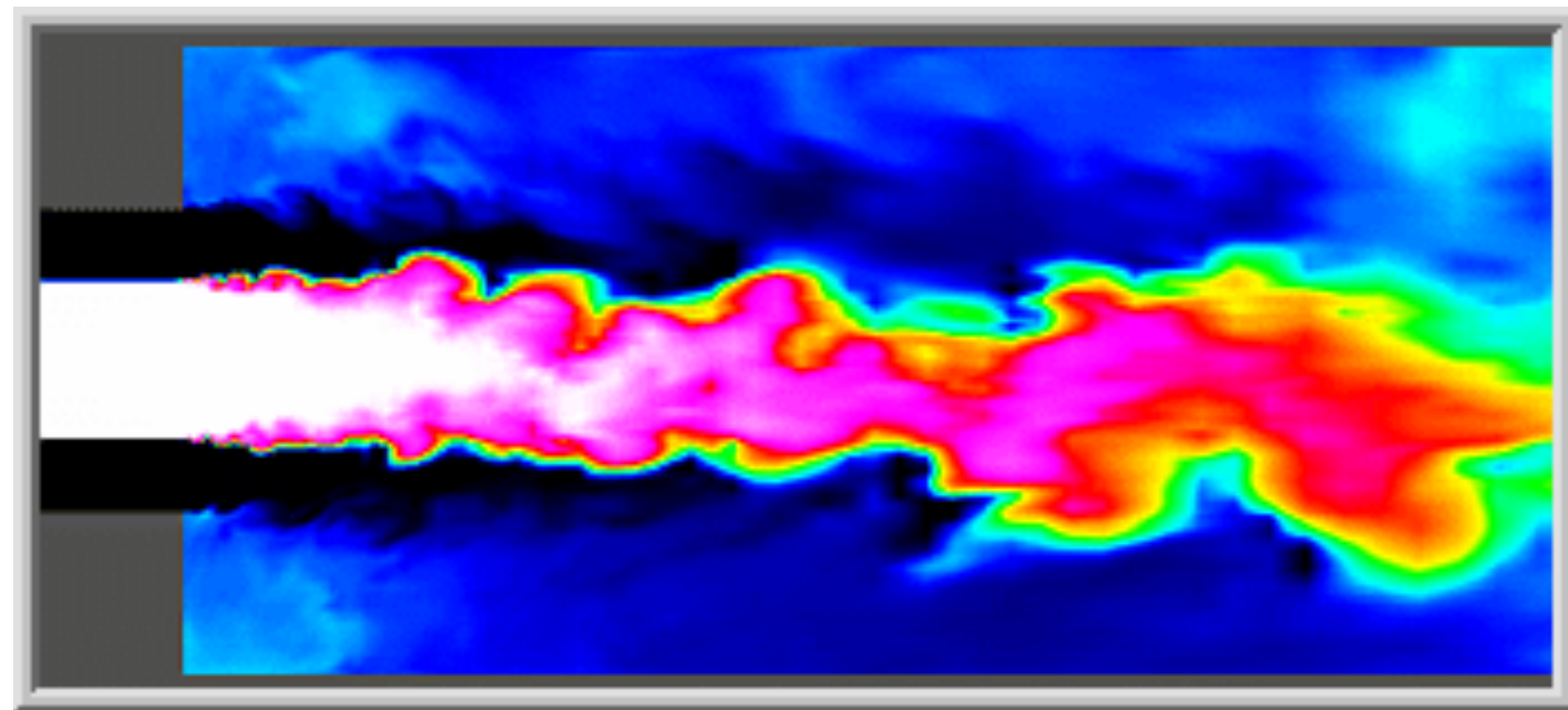
Table 4: The dispersion relation suggests new PIGM

Physics	PDE	Dispersion Relation
Mixed diffusion Poisson	$a\phi_{tt} - b\phi_t + \nabla^2\phi = 0$ ($a > 0, b > 0$)	$\omega = \frac{i}{2a}(b \pm \sqrt{b^2 + 4ak^2})$
Fractional diffusion	$\phi_t + (-\Delta)^\beta\phi = 0$ ($\beta > 0$)	$\omega = -ik^{2\beta}$
Third-order “diffusion”	$\phi_{ttt} - \Delta u = 0$	$\omega = (-i, e^{i\frac{\pi}{6}}, e^{i\frac{5\pi}{6}})k^{\frac{2}{3}}$
Elasticity (Biharmonic)	$\phi_t + \nabla^2\nabla^2\phi = 0$	$\omega = -ik^4$

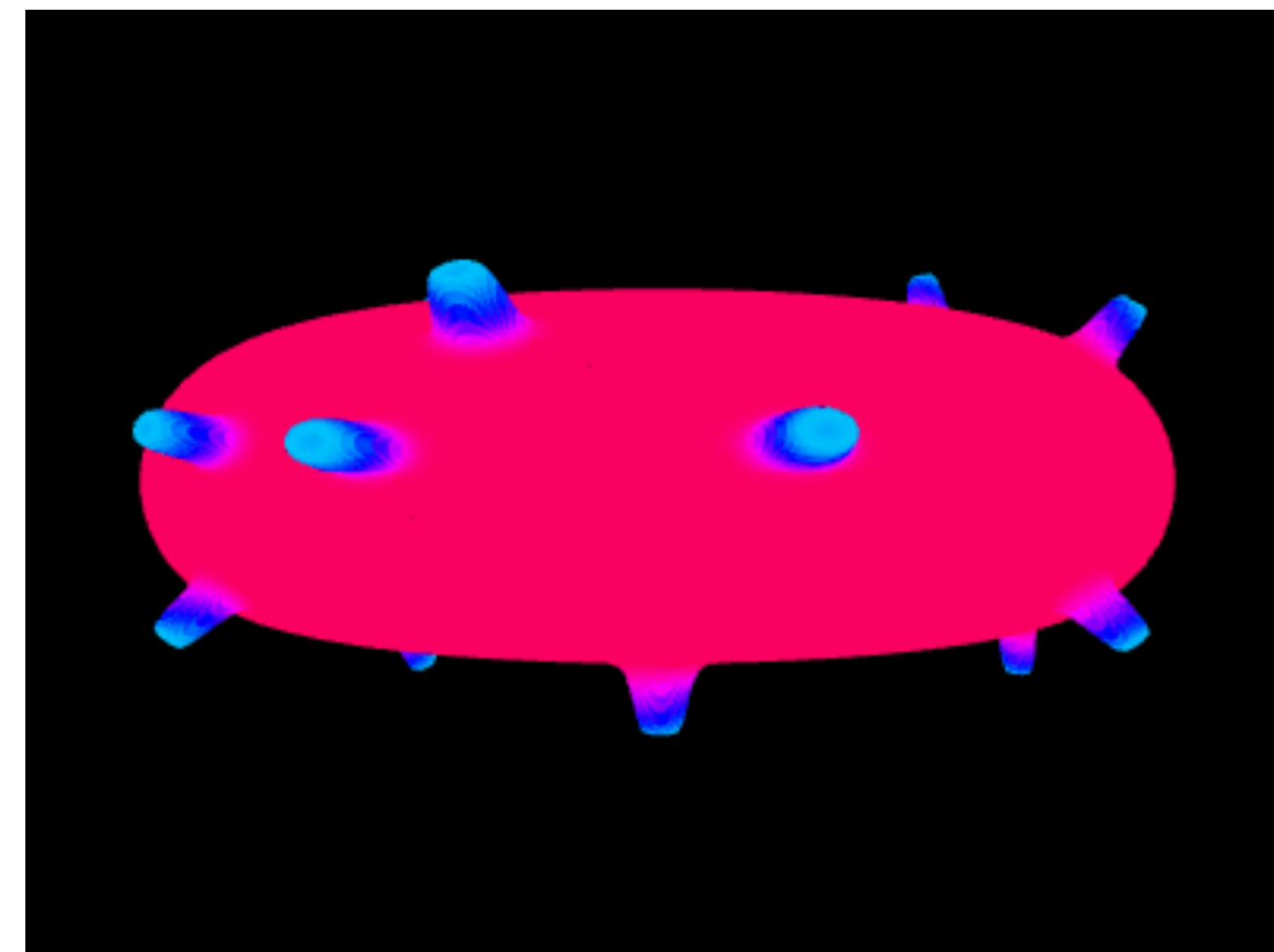
Open Questions

- Among s-generative PDEs, which one gives the best performance (in theory and in practice)?
- Going beyond smooth and linear PDEs. E.g., Navier-Stokes equation, reaction-diffusion equation

Navier-Stokes equation



Reaction-diffusion equation



Thank you for your listening!