

# Arbitrarily-Conditioned Multi-Functional Diffusion for Multi-Physics Emulation

ICML 2025

基于任意条件的多函数扩散模型的多物理场模拟方法

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# Background & Motivation

核心任务：捕获多物理场系统之间各个函数的关系，执行多种任务（正向预测、反向推断、函数模拟）

## 传统物理模拟方法

eg:有限元 有限差分

优点：

理论严谨，结果可靠  
能严格满足物理方程约束

缺点：

计算成本极高（如计算大型矩阵）  
多物理场的系统更加复杂！  
仿真一次流体可能耗时数小时甚至数天！

VS

## 现代机器学习代理模型

eg:FNO PINN

优点：

推理速度快  
相比传统方法能降低计算成本

缺点：

不同任务需要单独训练模型  
不支持不确定性量化

# 核心贡献

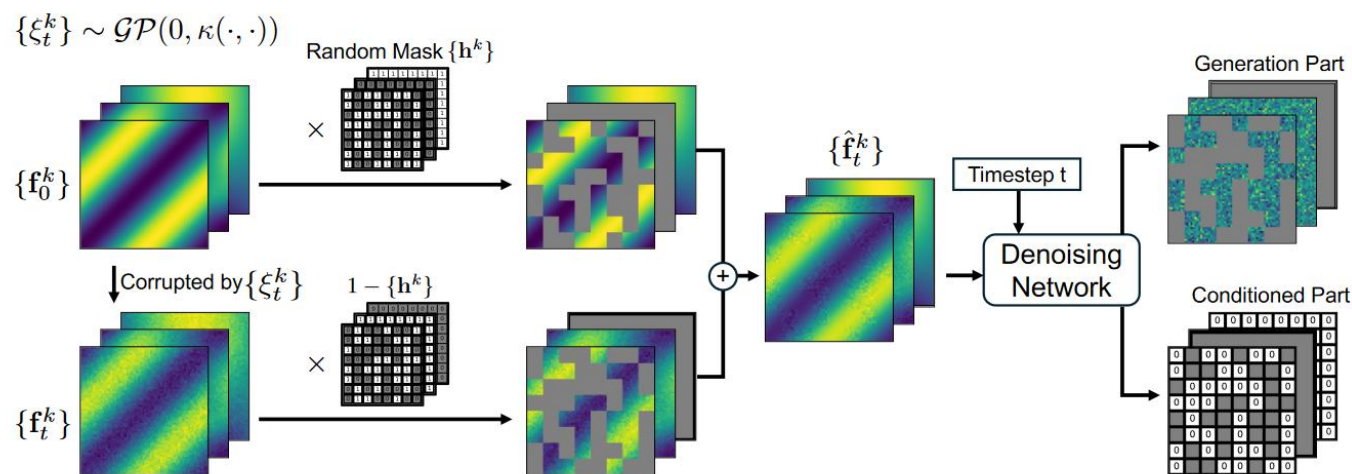
## 1. 多功能扩散模型

DDPM扩展到函数空间，用高斯过程建模噪声函数

$$f_t(\cdot) = \sqrt{\hat{\alpha}_t} f_0(\cdot) + \sqrt{1 - \hat{\alpha}_t} \xi_t(\cdot) \quad \xi_t \sim \mathcal{GP}(\cdot | 0, \kappa(\mathbf{z}, \mathbf{z}'))$$

## 2. 任意条件去噪损失

随机掩码策略，灵活处理条件生成



## 3. 高效训练与采样

分解核函数，使用克罗内克积，避免计算大型矩阵

(参考知乎小小将《扩散模型之DDPM》)

# DDPM



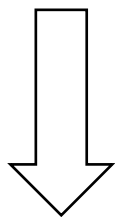
随机噪声  $\xi$   $\longrightarrow$  样本数据  $x$

加噪  $x_0 \rightarrow x_1 \rightarrow x_2 \rightarrow x_3 \rightarrow \dots \rightarrow x_T$

去噪  $x_T \rightarrow x_{T-1} \rightarrow x_{T-2} \rightarrow x_{T-3} \rightarrow \dots \rightarrow x_0$

加噪建模  $x_t = \sqrt{\alpha_t}x_{t-1} + \sqrt{\beta_t}\epsilon_t, \epsilon_t \sim \mathcal{N}(0, I)$

迭代  $x_{t-1} = \sqrt{\alpha_{t-1}}x_{t-2} + \sqrt{\beta_{t-1}}\epsilon_{t-1}, \epsilon_{t-1} \sim \mathcal{N}(0, I)$



$$x_t = \sqrt{\alpha_t}x_0 + \sqrt{\beta_t}\epsilon, \epsilon \sim \mathcal{N}(0, I)$$

$$x_0 = \frac{1}{\sqrt{\alpha_t}}(x_t - \sqrt{\beta_t}\epsilon)$$

令T步后  $\bar{\alpha}_T \approx 0$  数据经加噪近似为高斯噪声

$$q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\alpha_t}x_0, (1 - \bar{\alpha}_t)I)$$

$$q(x_{t-1}|x_t) \rightarrow q(x_{t-1}|x_t, x_0) = \mathcal{N}(x_{t-1}; \widehat{\mu}(x_t, x_0), \widehat{\beta}_t I)$$

$$q(x_{t-1}|x_t, x_0) = q(x_t|x_{t-1}, x_0) \frac{q(x_{t-1}|x_0)}{q(x_t|x_0)}$$

$$\widehat{\mu}(x_t, x_0) = \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t}x_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1 - \bar{\alpha}_t}x_0$$

$$\widehat{\beta}_t = \frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t}\beta_t$$

用  $x_t$  估计  $x_0$  ?

$$\mu(x_t) = \frac{1}{\sqrt{\alpha_t}}(x_t - \sqrt{\beta_t}\epsilon_\theta(x_t, t))$$

$$\|x_0 - \mu(x_t)\|^2 = c \|\epsilon - \epsilon_\theta(\sqrt{\alpha_t}x_0 + \sqrt{\beta_t}\epsilon, t)\|^2$$

随机噪声 $\xi$   $\longrightarrow$  样本数据 $x$

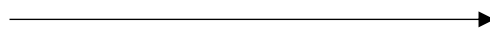
$x$ 是函数形式? 对函数的扩散

$$x_t = \overline{\alpha}_t x_0 + \overline{\beta}_t \overline{\varepsilon}_t, \quad \overline{\varepsilon}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \quad \longrightarrow \quad f_t = \overline{\alpha}_t f_0 + \overline{\beta}_t \overline{\varepsilon}_t, \quad \overline{\varepsilon}_t \sim \overset{\text{高斯过程}}{\mathcal{GP}}(\mathbf{0}, \mathcal{K}(\mathbf{z}, \mathbf{z}'))$$

原数据  $\xrightarrow{\text{加噪}}$  高斯噪声

原函数  $\xrightarrow{\text{加噪}}$  噪声函数

$$\varepsilon_{\theta}(x_t, t)$$



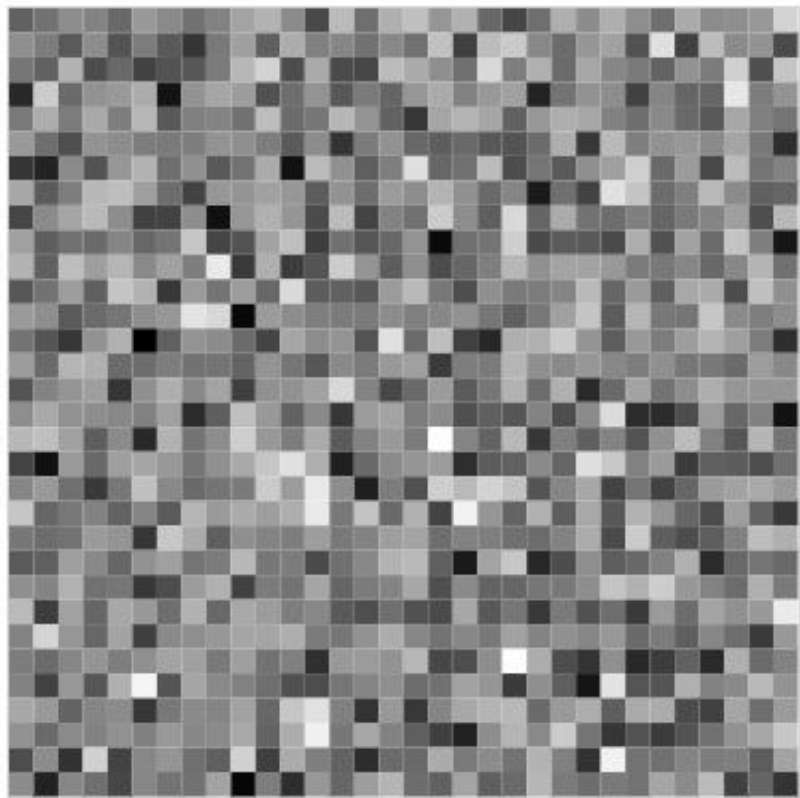
$$\varepsilon_{\theta}(f_t, t, \mathbf{z})$$

M个物理场



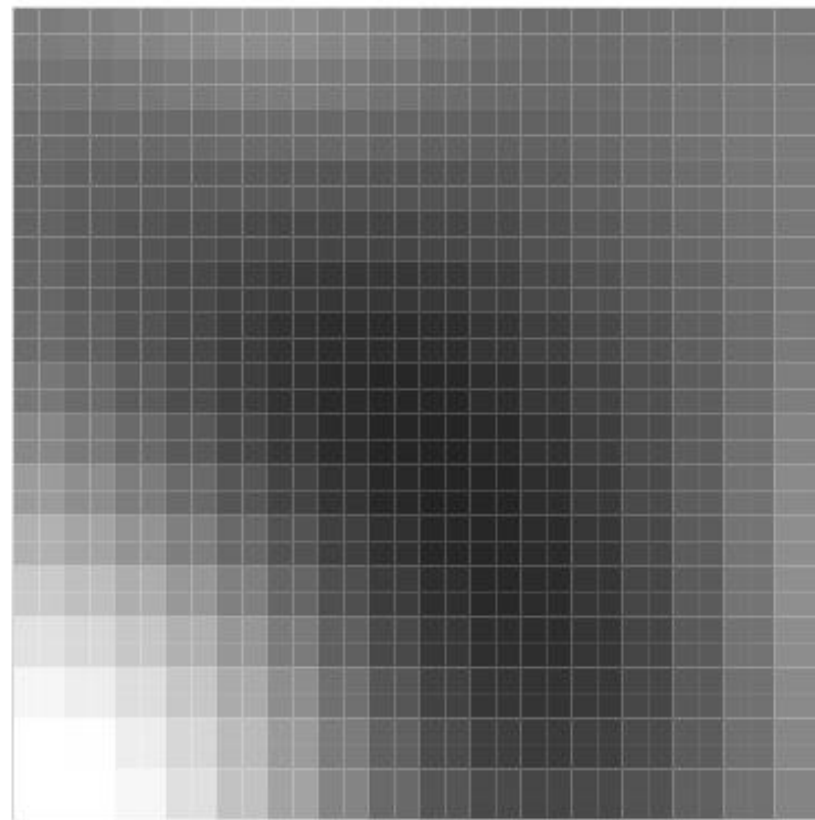
$$\varepsilon_{\theta}(f_t^1, f_t^2, \dots, f_t^M, t, \mathbf{z}) \xrightarrow{\text{预测}} \varepsilon_t^1, \varepsilon_t^2, \dots, \varepsilon_t^M$$

普通高斯噪声



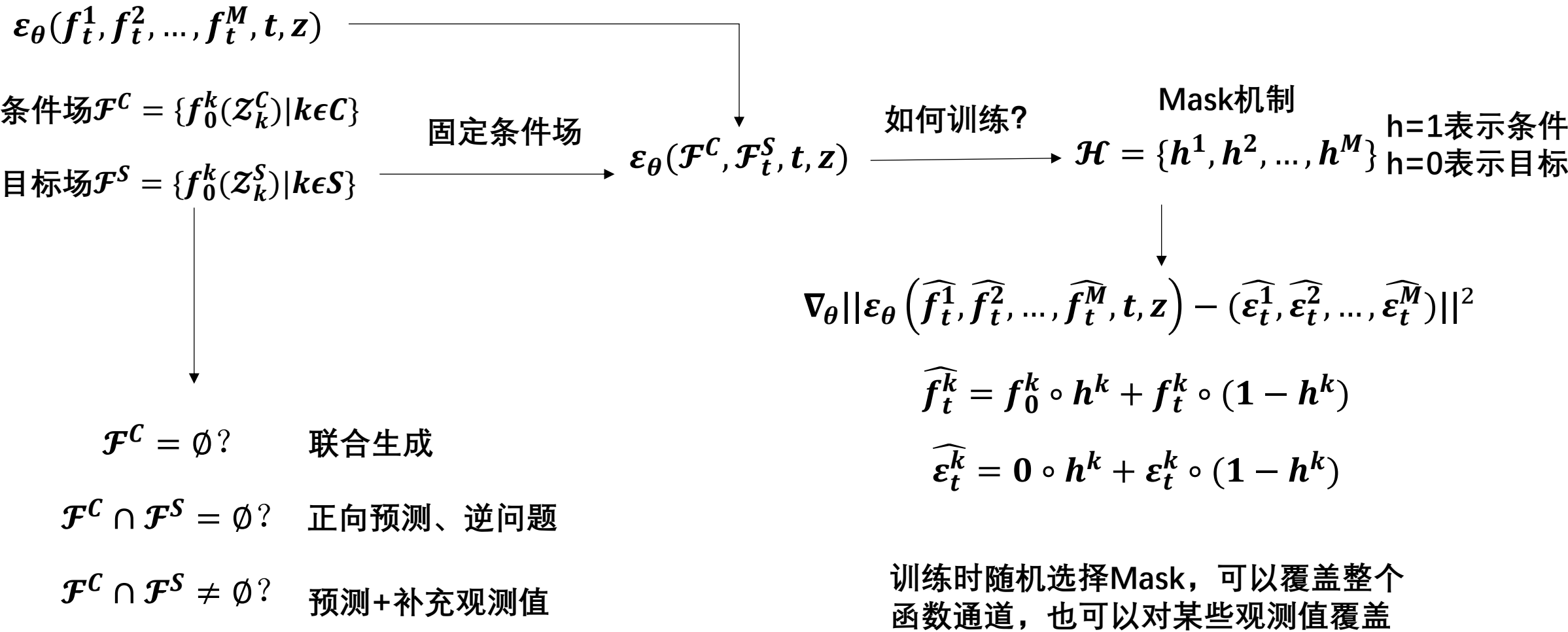
每个位置都完全独立

高斯过程噪声



$\bar{\epsilon}_t \sim \mathcal{GP}(0, \mathcal{K}(z, z'))$  空间关联

M个物理场，有作为条件的，也有生成的目标



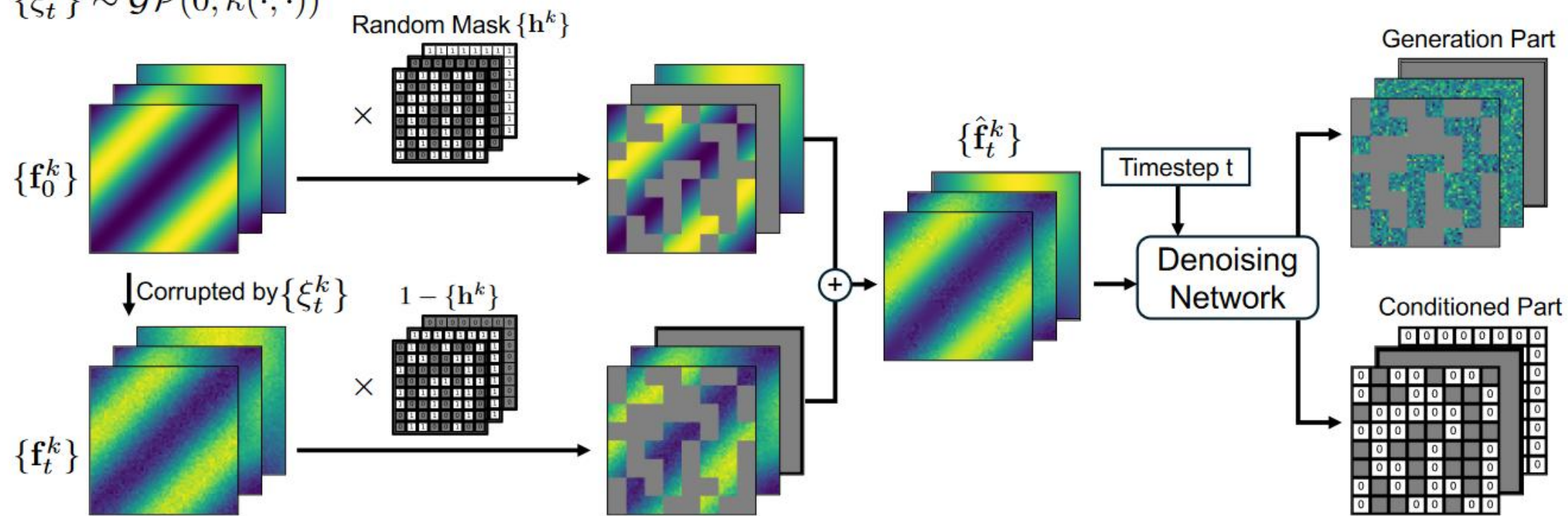
$\mathcal{F}^C = \emptyset?$  联合生成

$\mathcal{F}^C \cap \mathcal{F}^S = \emptyset?$  正向预测、逆问题

$\mathcal{F}^C \cap \mathcal{F}^S \neq \emptyset?$  预测+补充观测值

变换条件场和目标场的地位达到不同目的

$$\{\xi_t^k\} \sim \mathcal{GP}(0, \kappa(\cdot, \cdot))$$



## 训练流程

- 1、样本 $\{f_0^1, f_0^2, \dots, f_0^M\}$  采样位置 $\{Z_k\}_{k=1}^M$
- 2、时间 $t(1 \text{ to } T)$
- 3、采样 $\{\varepsilon_t^1, \varepsilon_t^2, \dots, \varepsilon_t^M\}$  对应 $f_t^K$
- 4、采样 $\{h_1, h_2, \dots, h_M\}$
- 5、 $\nabla_{\theta} ||\varepsilon_{\theta}(\widehat{f}_t^1, \widehat{f}_t^2, \dots, \widehat{f}_t^M, t, z) - (\widehat{\varepsilon}_t^1, \widehat{\varepsilon}_t^2, \dots, \widehat{\varepsilon}_t^M)||^2$
- 6、循环收敛

## 采样流程

条件场 $\mathcal{F}^C$   
目标场 $\mathcal{F}^S$

- 1、Z上采样高斯过程 $\varepsilon$
- 2、求子集 $\varepsilon$  得到初始值 $\mathcal{F}_T^S$
- 3、from  $t=T \cdots 1$ , do  
    若 $t>1$   
        Z上采样高斯过程 $\varepsilon$   
        求子集得到 $\bar{\varepsilon}$   
 $\varepsilon_t = \varepsilon_{\theta}(\mathcal{F}^C \cup \mathcal{F}_t^S, t, Z)$   
        求子集 $\varepsilon_t$ 得到 $\varepsilon_t^S$   
$$\mathbf{F}_{t-1}^s = \frac{1}{\sqrt{1 - \beta_t}} \left( \mathbf{F}_t^s - \frac{\beta_t}{\sqrt{1 - \hat{\alpha}_t}} \bar{\xi}_t^s \right) + \sqrt{\hat{\beta}_t} \bar{\varepsilon}$$
- 4、return  $\mathcal{F}_0^S$

D-F  
Darcy-Flow

$$\begin{aligned} -\nabla \cdot (a(\mathbf{x}) \nabla u(\mathbf{x})) &= f(\mathbf{x}) \quad \mathbf{x} \in (0, 1)^2 \\ u(\mathbf{x}) &= 0, \quad \mathbf{x} \in \partial(0, 1)^2, \end{aligned} \quad (a, f, u)$$

C-D  
Convection Diffusion

$$\frac{\partial u(x, t)}{\partial t} + \nabla \cdot (v(x, t) u(x, t)) = D \nabla^2 u(x, t) + s(x, t), \quad (v, s, u)$$

D-R  
Diffusion Reaction

$$\begin{aligned} \frac{\partial v_1}{\partial t} &= D_1 \frac{\partial^2 v_1}{\partial x^2} + D_1 \frac{\partial^2 v_1}{\partial y^2} + v_1 - v_1^3 - k - v_2, & f_1 &= v_1(2.5, x, y) \\ \frac{\partial v_2}{\partial t} &= D_2 \frac{\partial^2 v_2}{\partial x^2} + D_2 \frac{\partial^2 v_2}{\partial y^2} + v_1 - v_2, & f_2 &= v_2(2.5, x, y) \\ & & u_1 &= v_1(5.0, x, y) \\ & & u_2 &= v_2(5.0, x, y) \\ & & & (f_1, f_2, u_1, u_2) \end{aligned}$$

T-F  
Torus Fluid

$$\begin{aligned} \frac{\partial w(\mathbf{x}, t)}{\partial t} + \mathbf{u} \cdot \nabla w(\mathbf{x}, t) &= \nu \nabla^2 w(\mathbf{x}, t) + f(\mathbf{x}), & \omega(x, t) & \quad t = 2, 4, 6, 8, 10 \\ w(\mathbf{x}, 0) &= w_0(\mathbf{x}), & & (\omega_0, \omega_t, f) \end{aligned}$$

## 实验结果（预测任务）

| Dataset | Task(s)             | ACM-FD                     | FNO                        | GNOT                       | DON                 | Simformer            |
|---------|---------------------|----------------------------|----------------------------|----------------------------|---------------------|----------------------|
| D-F     | $f, u$ to $a$       | <b>1.32e-02 (2.18e-04)</b> | 1.88e-02 (1.66e-04)        | 1.35e-01 (6.57e-05)        | 2.38e-02 (3.45e-04) | 1.18e-01 (3.00e-03)  |
|         | $a, u$ to $f$       | <b>1.59e-02 (1.59e-04)</b> | 2.37e-02 (1.87e-04)        | 1.00e+00 (0.00e+00)        | 3.76e-02 (7.75e-04) | 4.11e-02 (2.87e-03)  |
|         | $a, f$ to $u$       | <b>1.75e-02 (4.16e-04)</b> | 6.29e-02 (4.18e-04)        | 6.09e-01 (2.40e-01)        | 6.05e-02 (7.17e-04) | 4.04e-02 (5.17e-03)  |
|         | $u$ to $a$          | <b>3.91e-02 (7.08e-04)</b> | 5.57e-02 (4.16e-04)        | 1.35e-01 (1.99e-04)        | 5.08e-02 (5.91e-04) | 1.44e-01 (4.23e-03)  |
|         | $u$ to $f$          | <b>3.98e-02 (6.45e-04)</b> | 5.50e-02 (5.47e-04)        | 9.99e-01 (7.48e-04)        | 6.46e-02 (1.13e-04) | 1.06e-01 (3.98e-03)  |
| C-D     | $s, u$ to $v$       | <b>2.17e-02 (4.53e-04)</b> | 4.50e-02 (3.89e-04)        | 3.26e-02 (3.41e-03)        | 3.64e-02 (5.07e-04) | 3.96e-01 (4.79e-02)  |
|         | $v, u$ to $s$       | <b>5.45e-02 (1.40e-03)</b> | 7.93e-02 (8.48e-04)        | 1.22e-01 (1.91e-03)        | 7.04e-02 (7.53e-04) | 5.76e-02 (7.10e-02)  |
|         | $v, s$ to $u$       | 1.60e-02 (2.15e-04)        | 7.26e-02 (2.16e-04)        | <b>5.80e-03 (1.51e-04)</b> | 7.86e-02 (7.42e-04) | 1.03e-01 (1.95e-02)  |
|         | $u$ to $v$          | <b>2.66e-02 (3.08e-04)</b> | 5.90e-02 (8.22e-04)        | 6.69e-02 (3.66e-03)        | 4.55e-02 (6.09e-04) | 5.108e-01 (7.56e-02) |
|         | $u$ to $s$          | <b>6.06e-02 (2.54e-04)</b> | 1.16e-01 (5.63e-04)        | 1.85e-01 (2.84e-03)        | 9.65e-02 (5.52e-04) | 9.21e-01 (1.00e-01)  |
| D-R     | $f_1, u_1$ to $f_2$ | 1.44e-02 (8.96e-04)        | <b>1.07e-02 (1.92e-04)</b> | 4.53e-01 (4.34e-02)        | 2.93e-01 (1.29e-03) | 3.39e-02 (2.97e-03)  |
|         | $f_1, u_1$ to $u_2$ | <b>1.59e-02 (3.68e-04)</b> | 2.02e-02 (2.42e-04)        | 3.91e-01 (1.86e-02)        | 2.03e-01 (2.22e-03) | 3.67e-02 (2.36e-03)  |
|         | $f_2, u_2$ to $f_1$ | <b>4.10e-02 (8.93e-04)</b> | 5.52e-02 (3.01e-03)        | 6.53e-01 (2.04e-02)        | 4.24e-01 (9.26e-04) | 1.21e-01 (3.11e-03)  |
|         | $f_2, u_2$ to $u_1$ | <b>5.86e-02 (3.43e-04)</b> | 7.82e-02 (1.29e-04)        | 4.88e-01 (2.92e-02)        | 2.98e-01 (2.61e-03) | 1.01e-01 (2.70e-03)  |
| T-F     | $w_0, w_5$ to $w_1$ | 2.73e-02 (4.78e-03)        | <b>1.28e-02 (2.38e-04)</b> | 2.40e-02 (8.74e-04)        | 6.32e-02 (2.72e-04) | 6.14e-02 (2.44e-03)  |
|         | $w_0, w_5$ to $w_2$ | 2.43e-02 (1.60e-03)        | <b>2.08e-02 (9.80e-05)</b> | 4.00e-02 (5.92e-04)        | 7.69e-02 (4.41e-04) | 6.99e-02 (2.18e-03)  |
|         | $w_0, w_5$ to $w_3$ | 2.43e-02 (3.17e-03)        | <b>2.33e-02 (1.83e-04)</b> | 4.74e-02 (1.23e-03)        | 7.34e-02 (2.88e-04) | 8.34e-02 (2.60e-03)  |
|         | $w_0, w_5$ to $w_4$ | 1.68e-02 (1.81e-03)        | <b>1.41e-02 (1.17e-04)</b> | 3.95e-02 (6.73e-04)        | 5.57e-02 (1.73e-04) | 9.75e-02 (3.93e-03)  |
|         | $w_0, w_5$ to $f$   | <b>1.63e-02 (1.49e-03)</b> | 1.79e-02 (3.04e-04)        | 5.91e-02 (4.01e-03)        | 4.77e-02 (5.56e-04) | 1.14e-01 (4.00e-03)  |
|         | $w_0, f$ to $w_1$   | 3.10e-02 (4.08e-03)        | <b>9.68e-03 (3.22e-04)</b> | 2.09e-02 (3.62e-04)        | 6.08e-02 (3.14e-04) | 6.06e-02 (2.03e-03)  |
|         | $w_0, f$ to $w_2$   | 3.28e-02 (4.79e-03)        | <b>1.70e-02 (3.51e-04)</b> | 4.15e-02 (8.21e-04)        | 7.73e-02 (6.18e-04) | 6.18e-02 (1.02e-03)  |
|         | $w_0, f$ to $w_3$   | 3.49e-02 (2.38e-03)        | <b>2.38e-02 (8.37e-05)</b> | 5.61e-02 (8.23e-04)        | 8.82e-02 (4.45e-04) | 5.67e-02 (1.83e-03)  |
|         | $w_0, f$ to $w_4$   | 3.34e-02 (3.87e-03)        | <b>3.10e-02 (1.26e-04)</b> | 6.97e-02 (1.62e-03)        | 1.02e-01 (7.28e-04) | 4.10e-02 (1.98e-03)  |
|         | $w_0, f$ to $w_5$   | <b>3.26e-02 (2.13e-03)</b> | 3.81e-02 (2.01e-04)        | 8.35e-02 (7.33e-04)        | 1.21e-01 (8.20e-04) | 1.18e-01 (4.15e-03)  |

## 实验结果（生成任务）

1000组函数平均误差

| System | Task(s)        | ACM-FD        | MFD           | $\beta$ -VAE |
|--------|----------------|---------------|---------------|--------------|
| D-F    | Equation Error | <b>0.0576</b> | 0.0584        | 0.265        |
|        | MRPD           | <b>1.15</b>   | 0.980         | 0.932        |
| C-D    | Equation Error | <b>0.114</b>  | 0.127         | 0.282        |
|        | MRPD           | <b>1.00</b>   | 0.971         | 0.879        |
| T-F    | Equation Error | 0.0273        | <b>0.0234</b> | 0.737        |
|        | MRPD           | 0.8042        | <b>0.9537</b> | 0.524        |

MRPD: Mean Relative Pairwise Distance  
平均相对成对距离：衡量数据生成多样性

## 实验结果（补全任务）

| Dataset | Task(s)  | ACM-FD          | MFD-Inpaint | Interp   |
|---------|----------|-----------------|-------------|----------|
| D-F     | <i>a</i> | <b>1.21e-02</b> | 7.94e-02    | 1.04e-01 |
|         | <i>f</i> | <b>1.23e-02</b> | 6.41e-02    | 6.98e-01 |
|         | <i>u</i> | <b>1.09e-02</b> | 2.71e-02    | 8.07e-01 |
| C-D     | <i>v</i> | <b>1.87e-02</b> | 4.71e-01    | 8.30e-01 |
|         | <i>s</i> | <b>3.39e-02</b> | 3.22e-01    | 6.49e-01 |
|         | <i>u</i> | <b>1.45e-02</b> | 3.47e-02    | 8.97e-01 |

# 实验结果（不确定性量化）

重复实验100个样本

| Dataset | Task          | Method    | 0.9          | 0.95         | 0.99         |
|---------|---------------|-----------|--------------|--------------|--------------|
| C-D     | $s, u$ to $v$ | ACM-FD    | <b>0.833</b> | <b>0.880</b> | <b>0.921</b> |
|         |               | Simformer | 0.736        | 0.814        | 0.871        |
|         | $v, u$ to $s$ | ACM-FD    | <b>0.766</b> | <b>0.842</b> | <b>0.913</b> |
|         |               | Simformer | 0.683        | 0.767        | 0.879        |
|         | $v, s$ to $u$ | ACM-FD    | <b>0.939</b> | <b>0.968</b> | <b>0.990</b> |
|         |               | Simformer | 0.695        | 0.771        | 0.858        |
|         | $u$ to $v$    | ACM-FD    | <b>0.821</b> | <b>0.870</b> | <b>0.922</b> |
|         |               | Simformer | 0.775        | 0.850        | 0.912        |
|         | $u$ to $s$    | ACM-FD    | <b>0.920</b> | <b>0.949</b> | <b>0.972</b> |
|         |               | Simformer | 0.716        | 0.773        | 0.823        |
| D-F     | $a, u$ to $f$ | ACM-FD    | <b>0.947</b> | <b>0.974</b> | <b>0.991</b> |
|         |               | Simformer | 0.829        | 0.895        | 0.950        |
|         | $a, f$ to $u$ | ACM-FD    | <b>0.985</b> | <b>0.994</b> | <b>0.998</b> |
|         |               | Simformer | 0.922        | 0.955        | <b>0.998</b> |
|         | $u$ to $f$    | ACM-FD    | 0.867        | 0.909        | 0.952        |
|         |               | Simformer | <b>0.918</b> | <b>0.953</b> | <b>0.980</b> |

$$ECP = \frac{1}{N_{\text{total}}} \sum_{i=1}^{N_{\text{total}}} \mathbb{I}(y_i \in C_\alpha)$$

## 附：加速采样高斯过程

### 1、一元高斯分布采样

$$x \sim \mathcal{N}(0, 1)$$

### 2、多元高斯分布采样

$$x \sim \mathcal{N}(0, \Sigma)$$

多变量不独立则不能直接分别采样独立高斯

相关性需要满足协方差矩阵 $\Sigma$



先采样  $z \sim \mathcal{N}(0, I)$

对  $\Sigma$  做Cholesky分解

$$\Sigma = LL^T$$

$$x = Lz$$

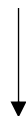
$$\text{Cov}(x) = E(xx^T) = LE(zz^T)L^T = LIL^T = \Sigma$$

### 3、高斯过程

$$f \sim \mathcal{N}(0, K)$$

在  $N$  个离散采样点上，为  $N$  维多元高斯

Cholesky分解时间复杂度 $O(N^3)!!$



尝试降维分解核函数

## 附：加速采样高斯过程

$$\kappa(x, x') = \sigma^2 \exp\left(-\frac{\|x - x'\|^2}{2\ell^2}\right)$$

$$\kappa(x, x') = \sigma^2 \exp\left(-\frac{(x_1 - x'_1)^2 + (x_2 - x'_2)^2}{2\ell^2}\right)$$

$$\kappa(x, x') = \sigma^2 \exp\left(-\frac{(x_1 - x'_1)^2}{2\ell^2}\right) \exp\left(-\frac{(x_2 - x'_2)^2}{2\ell^2}\right)$$

$$\kappa(x, x') = \kappa_1(x_1, x'_1) \kappa_2(x_2, x'_2)$$

$$\rightarrow K = K_1 \otimes K_2 \quad \text{克罗内克积}$$

$$\Sigma = LL^T = (L_1 \otimes L_2)(L_1 \otimes L_2)^T$$

$$K = K_1 \otimes K_2 \otimes K_3 \otimes \dots \otimes K_D$$

$$K^{-1} = (L_1^{-1})^T L_1^{-1} \otimes \dots \otimes (L_D^{-1})^T L_D^{-1} = A^T A$$

$$A = L_1^{-1} \otimes \dots \otimes L_D^{-1}$$

$$\text{vec}(\varepsilon_t) = A^T \eta, \quad \eta \sim \mathcal{N}(0, I)$$

实际操作

1、重塑  $\eta$  to  $\Pi = \text{tensor}(m_1 \times \dots \times m_D)$

2、 $\varepsilon_t = \Pi \times_1 L_1^{-1} \times_2 \dots \times_D L_D^{-1}$  模式乘

恳请批评指正

## 附：高斯过程

无限元高斯分布（高斯过程）

$$f(\mathbf{x}) \sim \mathcal{N}(\boldsymbol{\mu}(\mathbf{x}), \kappa(\mathbf{x}, \mathbf{x}))$$

一元高斯分布

$$p(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right)$$

$$\begin{bmatrix} f(\mathbf{x}) \\ \mathbf{y}^* \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_f \\ \boldsymbol{\mu}_y \end{bmatrix}, \begin{bmatrix} K_{ff} & K_{fy} \\ K_{fy}^T & K_{yy} \end{bmatrix}\right)$$

其中  $K_{ff} = \kappa(\mathbf{x}, \mathbf{x})$ ,  $K_{fy} = \kappa(\mathbf{x}, \mathbf{x}^*)$ ,  $K_{yy} = \kappa(\mathbf{x}^*, \mathbf{x}^*)$ , 则有

$$f \sim \mathcal{N}(K_{fy}^T K_{ff}^{-1} \mathbf{y} + \boldsymbol{\mu}_f, K_{yy} - K_{fy}^T K_{ff}^{-1} K_{fy})$$

多元高斯分布

$$p(\mathbf{x}) = (2\pi)^{-\frac{n}{2}} |\mathbf{K}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \mathbf{K}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right)$$

$$\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{K})$$