GenCP: Towards Generative Modeling Paradigm of Coupled Physics

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Outline

Introduction

Why multi-physics simulation is vital.

Why multi-physics simulation is difficult.

Approach

How to learn decoupled physics.

How to infer coupled physics.

How to understand GenCP theoretically.

Results

Synthetic data

Fluid structure interaction setting

Nuclear thermal coupling setting

Introduction

Multi-physics simulation is a critical and ubiquitous problem in science and engineering, since real-world systems often involve **strongly coupled multi-physics interactions**.

Coupling Type	Physical Fields	Representative Applications
Fluid–Structure Interaction	Fluid dynamics + Structural mechanics	Aeroelastic flutter of aircraft wings; heart valve dynamics; wind-induced bridge response; MEMS micropumps; submarine hull vibration
Fluid–Thermal Coupling	Fluid flow + Heat transfer	Electronics cooling; HVAC system design; combustion chamber simulation; solar collectors; nuclear reactor cooling loops
Neutron–Thermal Coupling	Neutron transport + Thermal analysis	Reactor core design (fission/fusion); fuel rod temperature prediction; reactor safety analysis; neutron-driven material heating (e.g., fusion blankets)
Electro–Thermal Coupling	Electromagnetics + Heat transfer	Chip/PCB thermal management; battery overheating protection; RF antenna heating; induction heating processes
Electro–Chemical–Thermal Coupling	Electrochemistry + Heat + Mass transport	Battery aging during charge/discharge; fuel cell optimization; electroplating and corrosion modeling

Motivation

- Accurate simulation is critical but:
  - ◦Coupled simulations are computationally expensive
  - ◦Available data is often decoupled (single-physics simulations)

How can we develop a framework that learns coupled physics from decoupled training data while ensuring high fidelity, efficiency, and reliability?

Core Challenges

- Training data is conditional (decoupled), while inference requires joint (coupled) distribution
- Strong coupling complexity, incoporating nonlinear & bidirectional interactions
- Efficiency (scalability) vs fidelity trade-off
- Lack of theoretical guarantees

Limitations of Existing Methods

- Traditional numerical solvers:
  Require fully coupled simulations, with high computational cost and limited scalability
- Operator learning / neural PDE methods:
  Limited to capture high-frequency, high-dimensional, and stochastic behaviors
- Generative models
  Typically model single-field distributions; Cannot directly bridge decoupled training to coupled generation

GenCP： Generative multi-physics simulation paradigm

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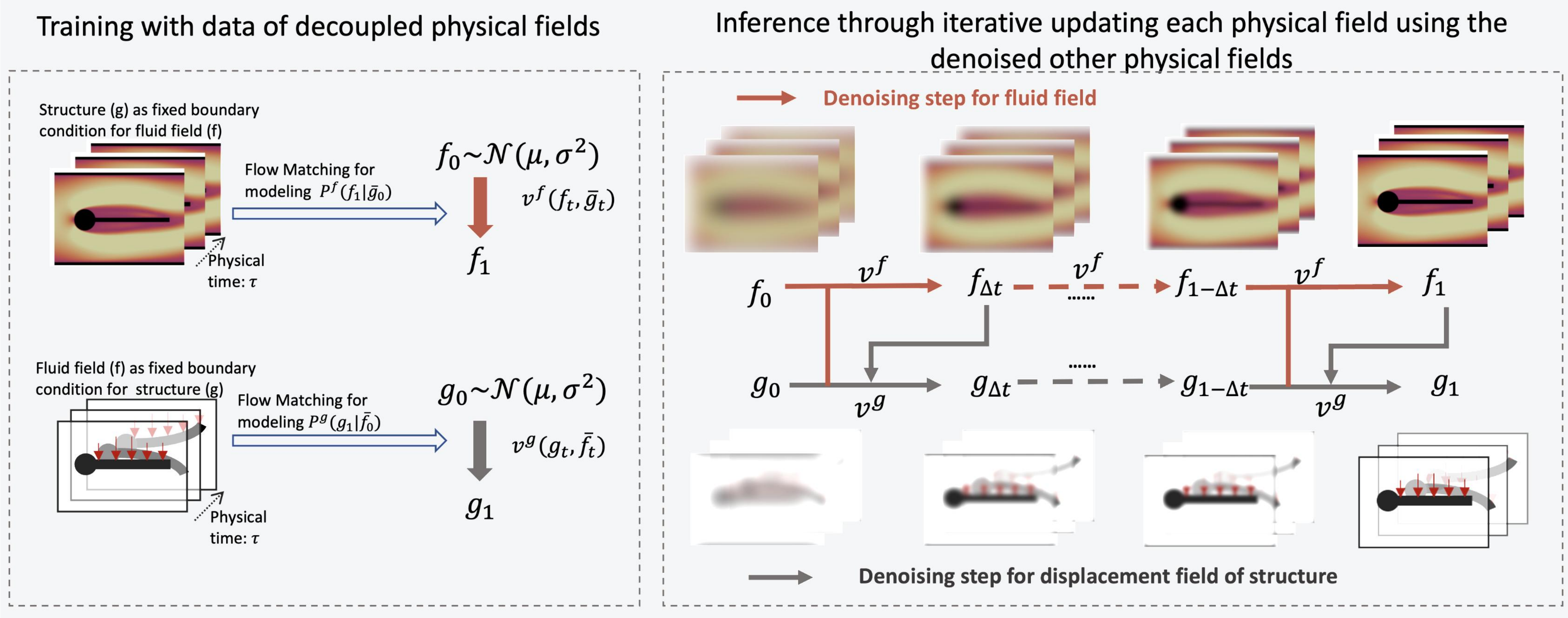
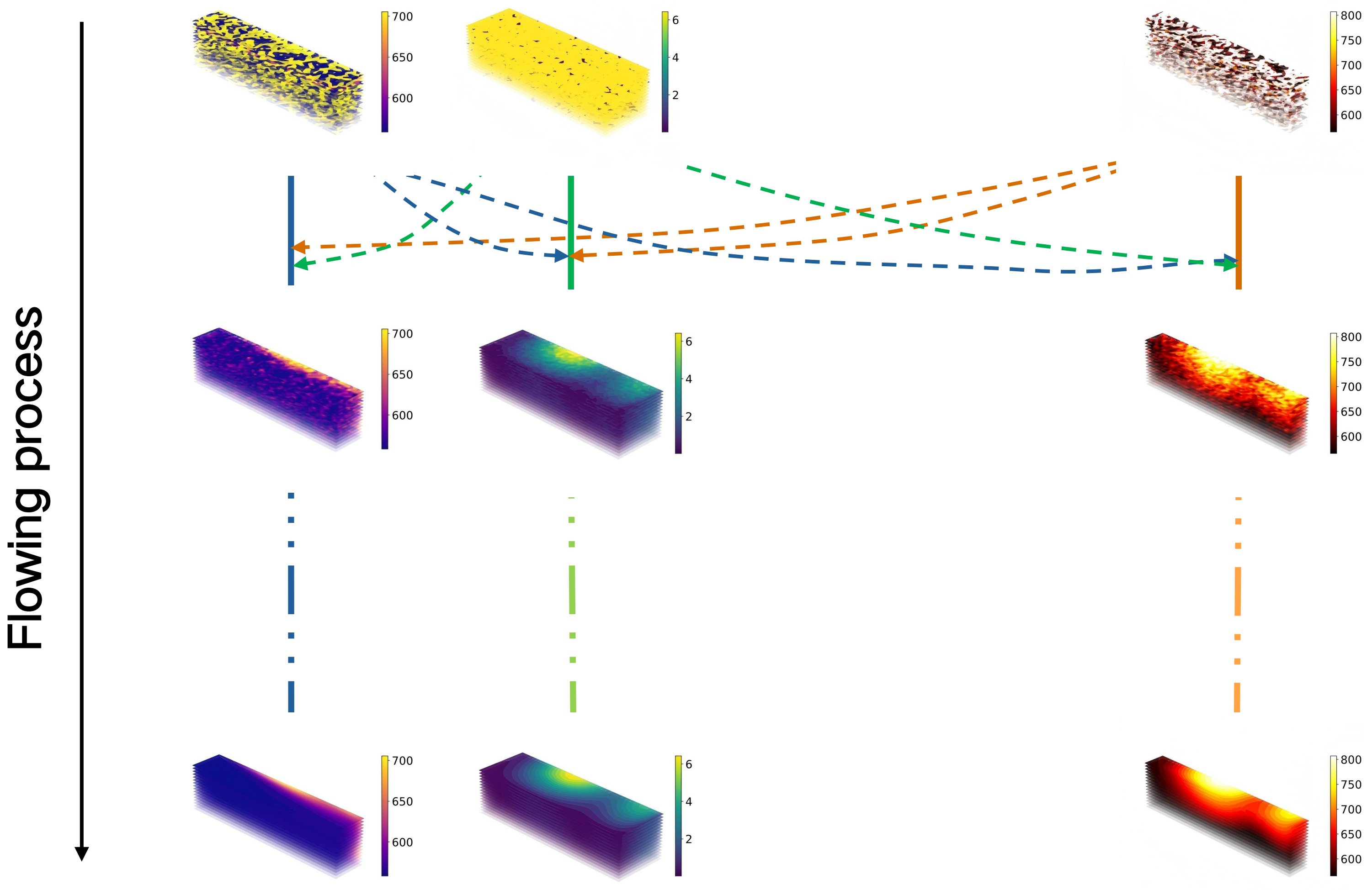


GenCP： Generative multi-physics simulation paradigm



Theoretical intuition & gurantee

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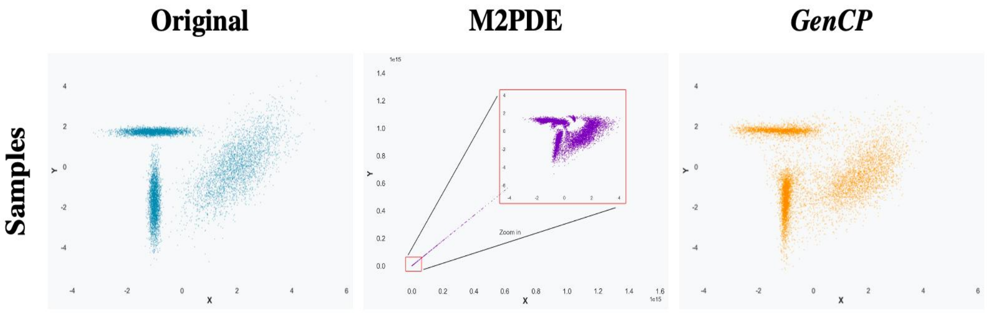
The transition from decoupled to coupled data can be understood, in a distributional sense, as **learning conditional distributions to enable joint sampling**.

We **evolve multi-physics fields in the latent space** of Flow Matching, and adopt an **operator-splitting scheme to achieve controllable sampling error**.

$$W_1\left(\mu_1^{(\tau,\text{learn})}, \mu_1\right) \le C_{\text{stab}}\left(\tau + \varepsilon_f + \varepsilon_g\right)$$



Weak continuity equation. Functional flow matching (FFM) (Kerrigan et al., 2023) models measure evolution directly via the weak continuity equation. For any smooth test function $\varphi : \mathcal{U} \to \mathbb{R}$,

$$\int_0^1 \int_{\mathcal{U}} \Big(\partial_t \varphi(u) + \langle D\varphi(u), v(t,u)\rangle_{\mathcal{U}}\Big)\, d\mu_t(u)\, dt = 0, \tag{1}$$

Decomposing the weak equation. To exploit the decoupled datasets we decompose $v(t,u) = v^{(f)}(t,u) + v^{(g)}(t,u), v^{(f)}(t,u) = (v_f(t,f,g), 0), v^{(g)}(t,u) = (0, v_g(t,f,g))$. Because the weak formulation is linear in v, we obtain

$$\int_0^1 \int_{\mathcal{U}} \big(\partial_t \varphi(u) + (\mathcal{L}_f(t) + \mathcal{L}_g(t))\varphi(u)\big)\, d\mu_t(u)\, dt = 0,$$

where the component Liouville operators are

$$\mathcal{L}_f(t)\varphi(u) := \langle v^{(f)}(t,u), D\varphi(u)\rangle_{\mathcal{U}}, \qquad \mathcal{L}_g(t)\varphi(u) := \langle v^{(g)}(t,u), D\varphi(u)\rangle_{\mathcal{U}}.$$

Lie–Trotter splitting. Let $S_{t+h\leftarrow t}$ denote the observable propagator defined by $(S_{t+h\leftarrow t}\varphi)(u) := \varphi(\Phi_{t+h\leftarrow t}(u))$, where $\Phi_{t+h\leftarrow t}$ is the flow map of v. At the observable level, $S_{t+h\leftarrow t} \approx S^{(g)}_{t+h\leftarrow t} \circ S^{(f)}_{t+h\leftarrow t}$, which by duality gives the measure-level approximation

$$\mu_{t+h} \;\approx\; \left(\Phi^{(g)}_{t+h\leftarrow t} \circ \Phi^{(f)}_{t+h\leftarrow t}\right)_{\#}\mu_t. \tag{2}$$

Learning objectives. Parameterize two operator-valued models $\hat{v}_f(f,g,t;\theta_f)$ and $\hat{v}_g(f,g,t;\theta_g)$ that map inputs (f_t, g_t, t) to elements of $\mathcal{F}$ and $\mathcal{G}$, respectively. Minimize the mean-square losses

$$\mathcal{L}_f(\theta_f) = \mathbb{E}_{t,(f_1,\bar{g})\sim\mathcal{D}_f,\, z_f, z_g}\left[\|v_f - \hat{v}_f(f_t, g_t, t;\theta_f)\|^2_{\mathcal{F}}\right], \tag{3}$$

$$\mathcal{L}_g(\theta_g) = \mathbb{E}_{t,(\bar{f},g_1)\sim\mathcal{D}_g,\, z'_f, z'_g}\left[\|v_g - \hat{v}_g(f_t, g_t, t;\theta_g)\|^2_{\mathcal{G}}\right]. \tag{4}$$

Algrithom: training and inference

Algorithm 1 Coupled Sampling via Lie–Trotter Splitting

```
Input: initial u_0 = (f_0, g_0), trained operators v̂_f, v̂_g, steps N
u ← u_0
for k = 0 to N − 1 do
    t ← k/N
    f ← f + τ v̂_f(f, g, t; θ_f)
    g ← g + τ v̂_g(f, g, t; θ_g)
    u ← (f, g)
end for
return u
```

Rollout with operator splitting

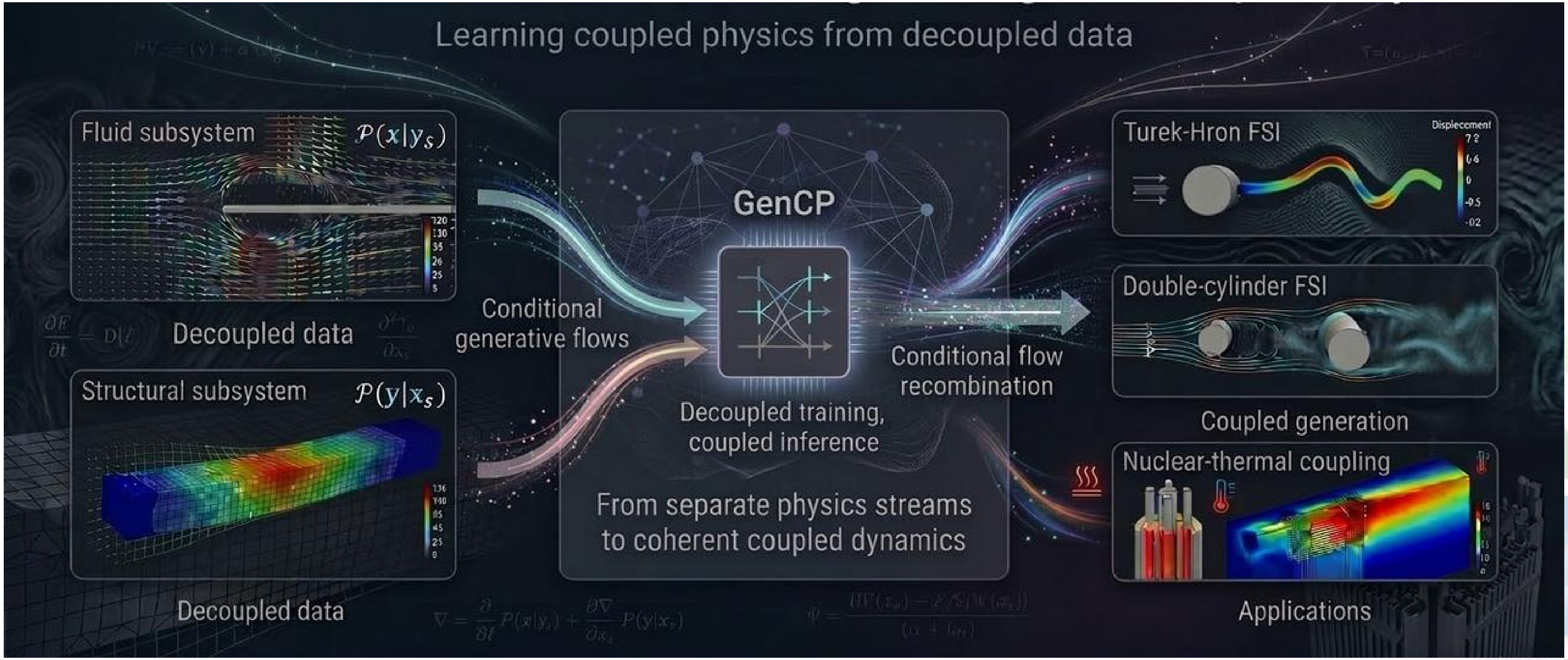
Algorithm 2 Training decoupled conditional velocity fields.

```
Input: decoupled datasets D_f, D_g
Initialize θ_f, θ_g
for epoch = 1 to E do
    for batch (f_1, g_0) ~ D_f do
        Sample t ~ U[0,1], z_f ~ π_F, z_g ~ π_G
        Compute f_t, g_t, ḟ_t and update θ_f to minimize ||ḟ_t − v̂_f(f_t, g_t, t; θ_f)||^2
    end for
    for batch (f_0, g_1) ~ D_g do
        Sample t ~ U[0,1], z'_f ~ π_F, z'_g ~ π_G
        Compute f_t, g_t, ġ_t and update θ_g to minimize ||ġ_t − v̂_g(f_t, g_t, t; θ_g)||^2
    end for
end for
```

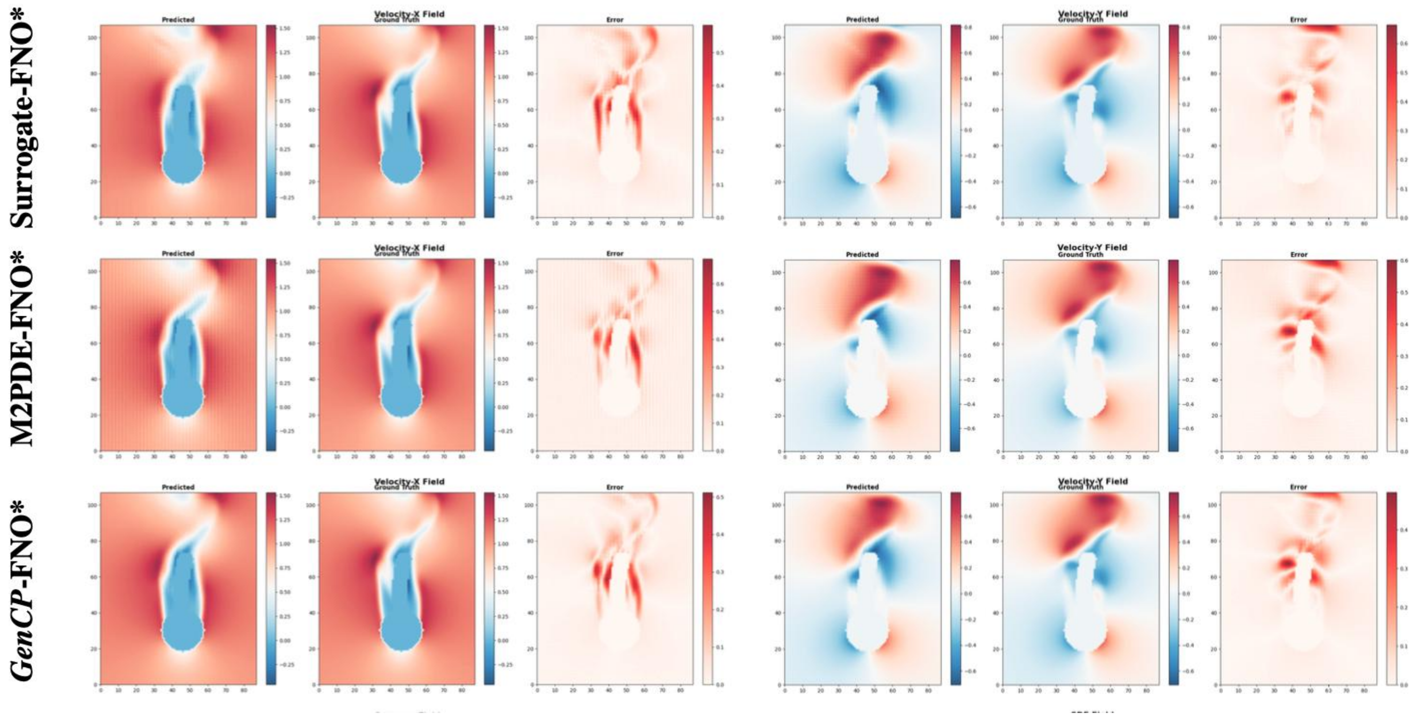
Single field training

Multi-physics problem statement

- Consider three **3D spatiotemporal** prediction problems under different physical scenarios, including:
- Field coupling interactions + Interface coupling interactions
- Weak coupling interactions + Strong coupling interactions

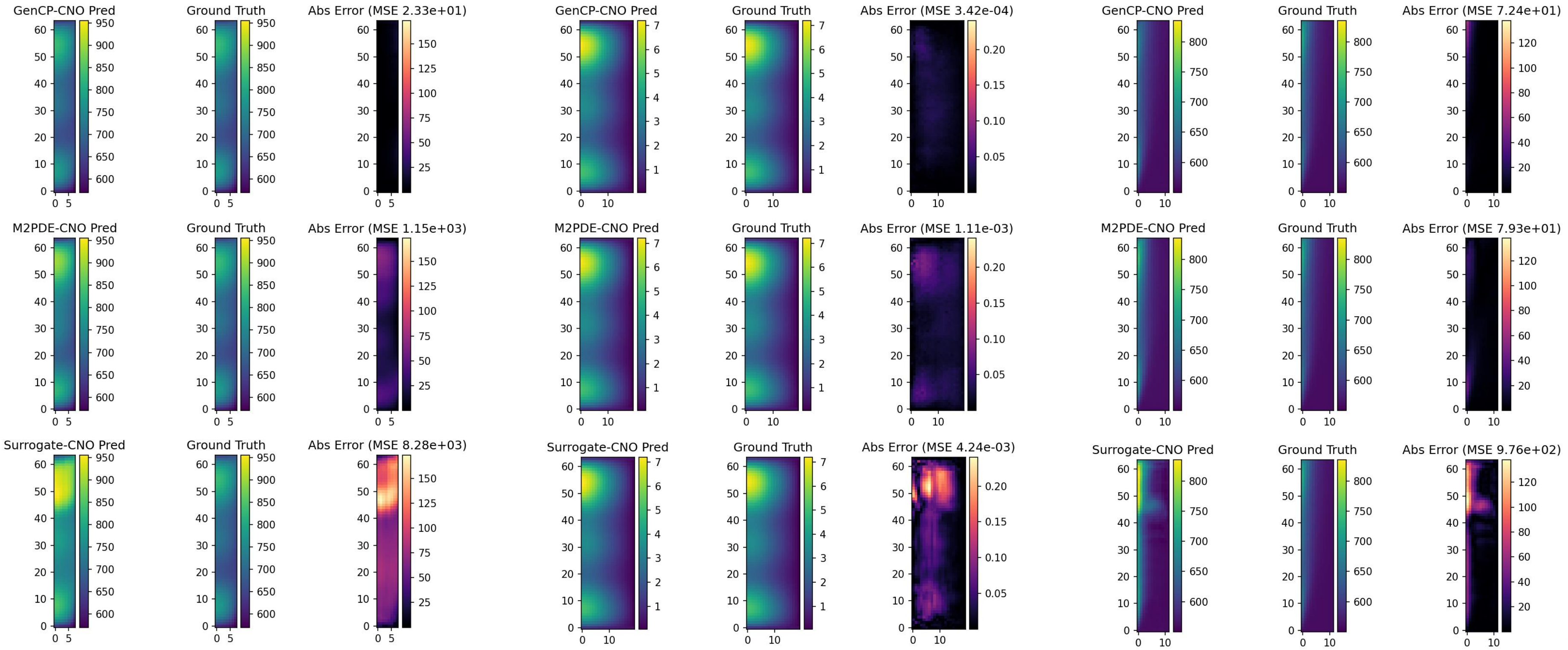


Experimental results: fluid-structure interaction



Rel L2 Norm Field	Validation on Decoupled Data u	 v	 p	 SDF	Test on Coupled Data u	 v	 p	 SDF	Inference Time
Joint Training	/	/	/	/	0.0088	0.03441	0.0544	0.0079	/
M2PDE-FNO*	0.0452	0.1582	0.1444	0.0206	0.0590	0.2415	0.2474	0.2482	277.20s
Surrogate-FNO*	0.0181	0.0756	0.0953	0.0087	0.0550	0.2257	0.2553	0.0112	93.20s
Our *GenCP*-FNO*	0.0091	0.0471	0.0548	0.0069	**0.0396**	**0.1678**	**0.1897**	**0.0081**	**19.50s**
M2PDE-CNO	0.0497	0.2075	0.3466	0.03937	0.05769	0.2809	0.4087	0.0390	347.00s
Surrogate-CNO	0.0204	0.0994	0.1526	0.0205	0.0469	0.1888	0.2278	0.0242	300.25s
Our *GenCP*-CNO	0.0150	0.0626	0.1187	0.0152	**0.0388**	**0.1821**	**0.2166**	**0.0183**	**16.25s**

Experimental results: nuclear-themal coupling



Fuel Neutron Fluid

Rel L2 Norm	Decoupled validation on decoupled data			Decoupled validation on coupled data			Coupled test on coupled data		
Field	Neutron	Fuel	Fluid	Neurton	Fuel	Fluid	Neurton	Fuel	Fluid
Our *GenCP*-FNO*	0.0022	0.0006	0.0038	0.0081	0.0371	0.0364	**0.0085**	**0.0364**	**0.0270**
Surrogate-FNO*	0.0086	0.0014	0.0032	0.0140	0.0167	0.0767	0.0149	0.0576	0.1095
M2PDE-FNO*	0.0052	0.0014	0.0018	0.0082	0.0085	0.0237	0.0136	0.1237	0.0463
Our *GenCP*-CNO	0.0024	0.0005	0.0110	0.0047	0.0083	0.0303	**0.0044**	**0.0105**	**0.0330**
Surrogate-CNO	0.0046	0.0007	0.0082	0.0073	0.0044	0.0567	0.0130	0.0553	0.3086
M2PDE-CNO	0.0053	0.0016	0.0092	0.0084	0.0017	0.0236	0.0164	0.0646	0.0401

Our group: AI for Scientific Simulation & Discovery Lab

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Paper: Tianrun Gao, Haoren Zheng, Wenhao Deng, Haodong Feng, Tao Zhang, Ruiqi Feng, Qianyi Chen, Tailin Wu. "GenCP: Towards Generative Modeling Paradigm of Coupled Physics." ICLR 2026

Code: https://github.com/AI4Science-WestlakeU/GenCP

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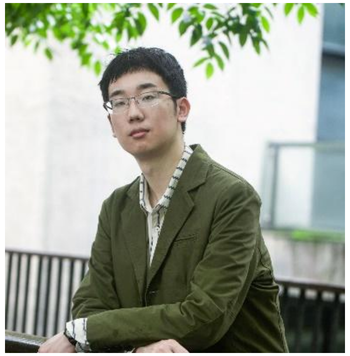

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Thank you!

Paper:

Group Website:

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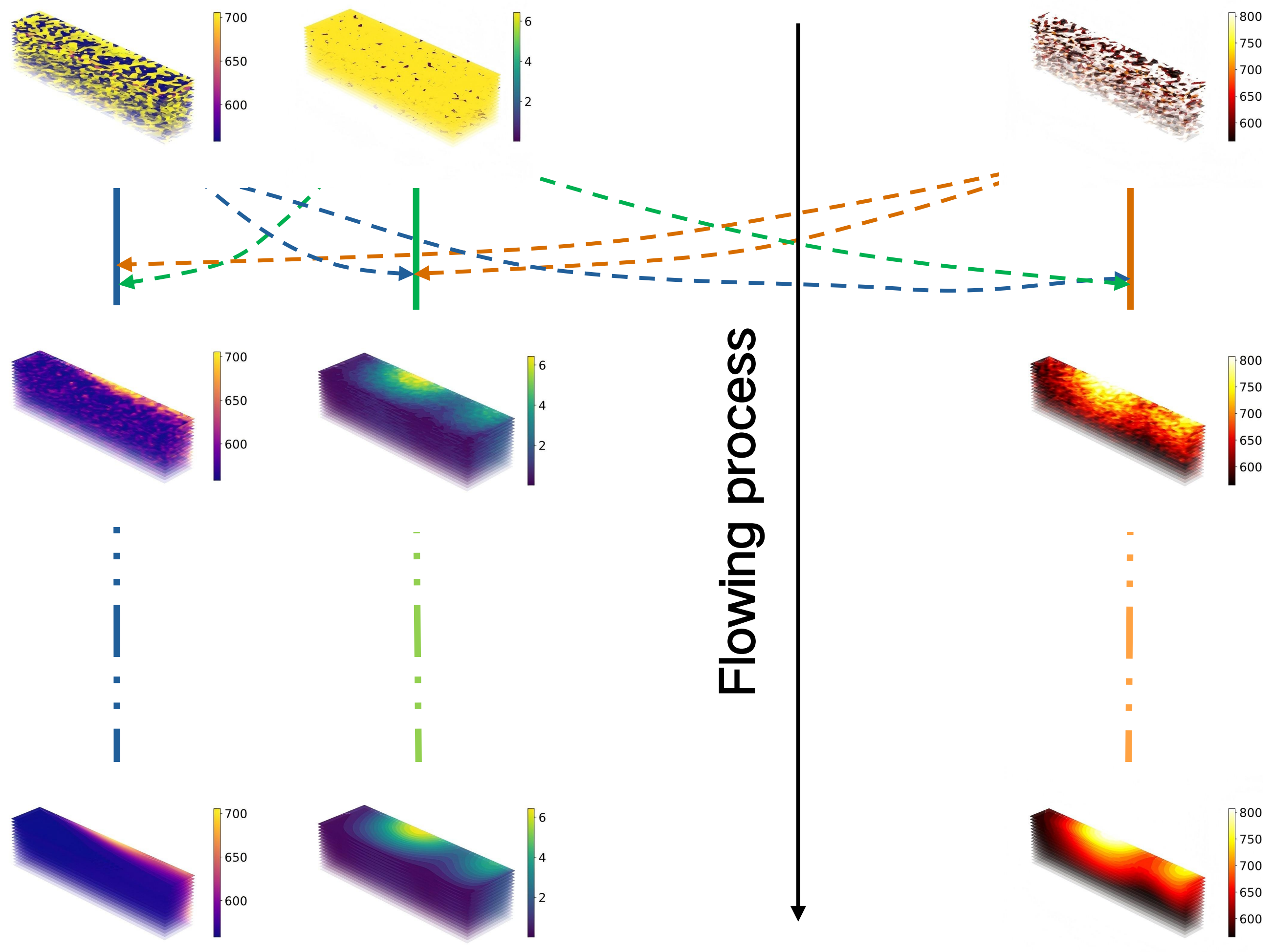
700
650
600
6
4
2
800
750
700
650
600
Flowing process