# **Compositional Generative Inverse Design**

Tailin Wu Assistant Professor of AI, Westlake University 02/19/2024 @ AI4Science Talks

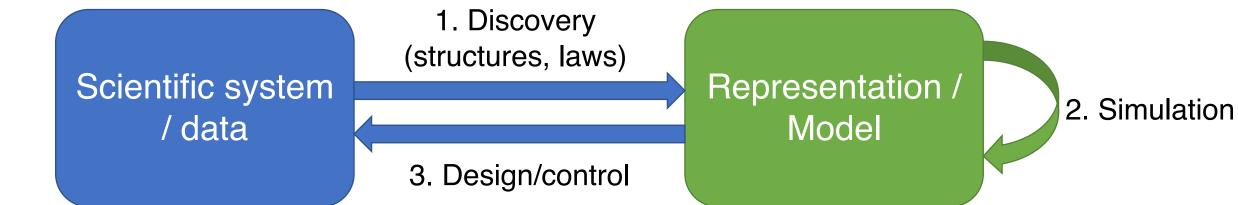
> **Collaborators:** Takashi Maruyama\* (NEC Laboratories Europe), Long Wei\*, Tao Zhang\* (Westlake U), Yilun Du\* (MIT), Gianluca laccarino, Jure Leskovec (Stanford)

\* denoes equal contributions

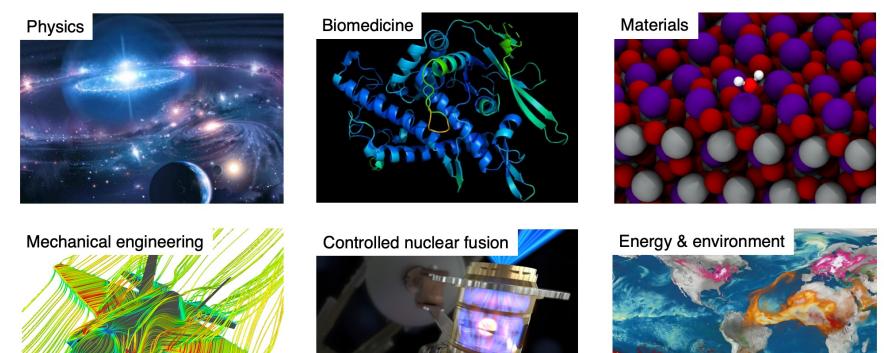
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Welcome collaborations! (more at the end)

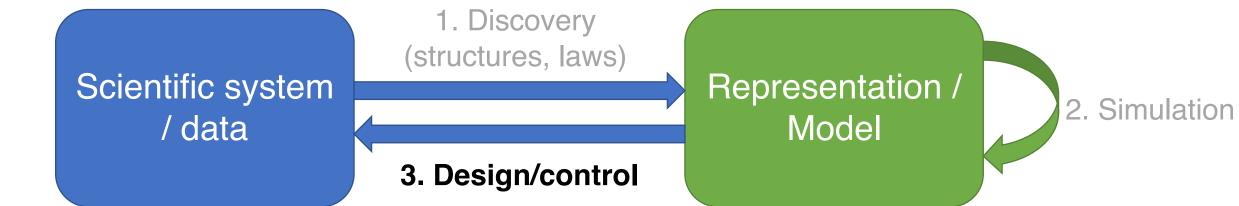
#### Al for Science:



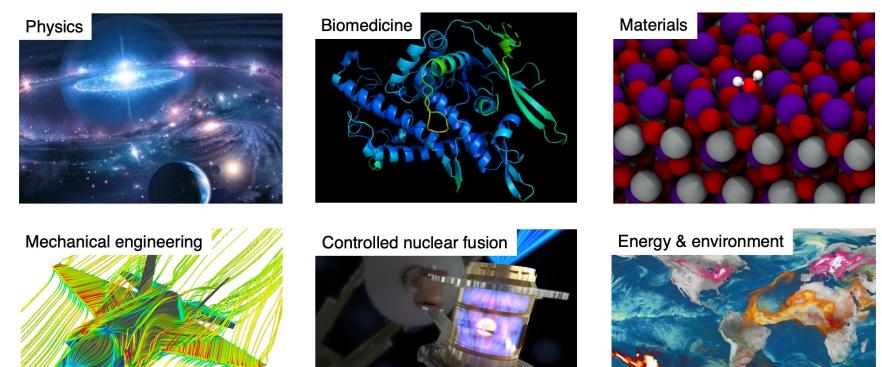
#### These three tasks are fundamental in science and engineering



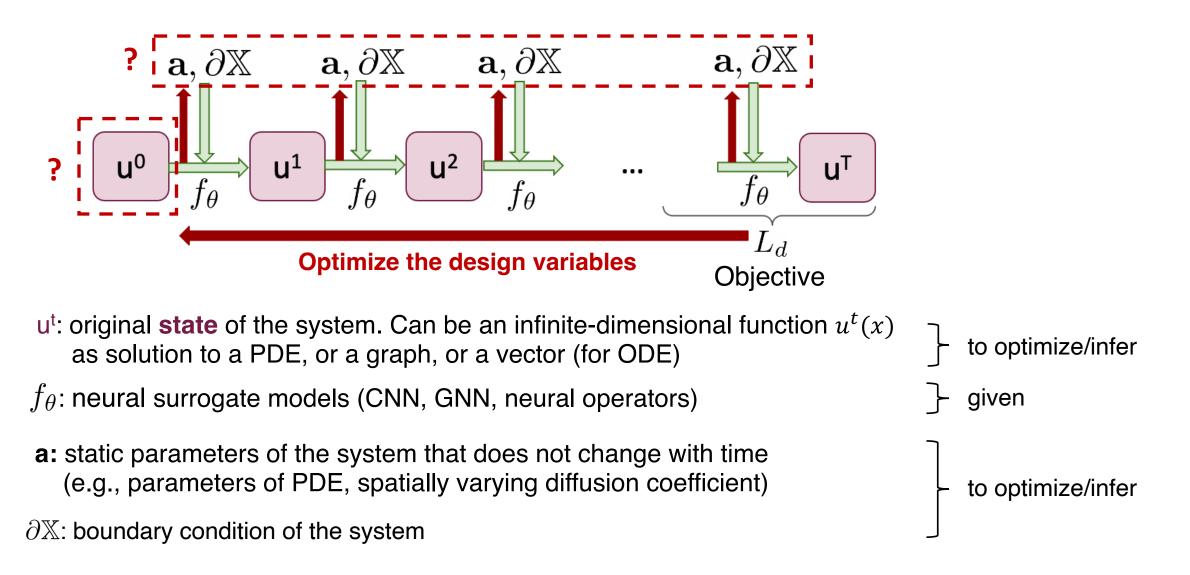
#### Al for Science:



#### These three tasks are fundamental in science and engineering



### Al for scientific design: definition

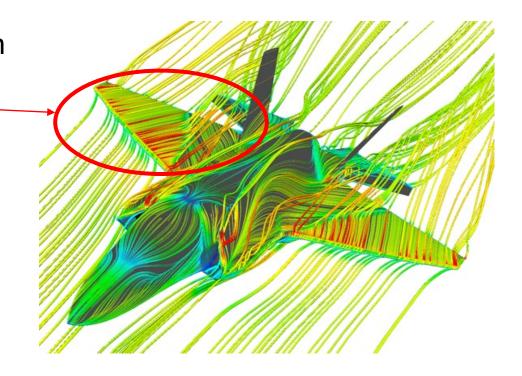


## Compositional inverse design: definition

Given objective  $J(U(\gamma), \gamma)$ , find design parameters  $\gamma$  that minimize J, where the parameters  $\gamma$  and/or the state U are more complex than in training.

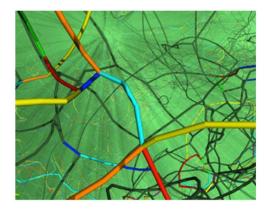
For example: **Training:** we only see how the fluid interacts with each <u>part</u> of the airplane

**Test:** design the <u>whole</u> airplane shape

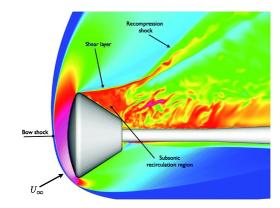


## Compositional inverse design: significance

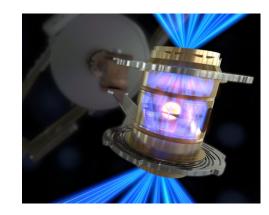
• Inverse design is **prevalent** in science and engineering:



materials science



Mechanical engineering



Controlled nuclear fusion

 Helps to explore continuous, high-dimensional design space, potential to find designs not imagined by humans

## Compositional inverse design: difficulty

#### • Complex design space:

- High Computational cost
- Complex composition relations

### Complex dynamics:

 How to characterize interaction between optimization of shape with physical process

### Generalization:

• How to generalize to more complex composition scenarios

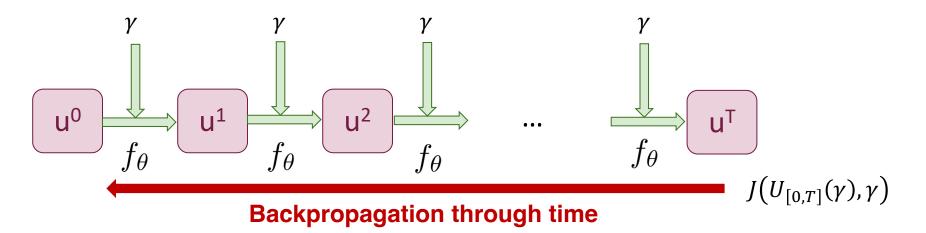
### Compositional inverse design: limitation of prior works

1. Traditional physical simulation methods (e.g., cross-entropy method):

- High accuracy but low efficiency
- Need rich expert knowledge
- Hard to deal with high-dimensional design space

## Compositional inverse design: limitation of prior works

#### 2. Recent methods using deep learning



- First, learn a surrogate forward model that autoregressively predict the dynamics  $U_{[0,T]}$  from the parameters  $\gamma$
- Then, using the objective  $J(U_{[0,T]}(\gamma), \gamma)$ , doing backpropagation and optimize  $\gamma$

<sup>[1]</sup> Allen, Kelsey R., et al. "Physical design using differentiable learned simulators." *NeurIPS* 2022

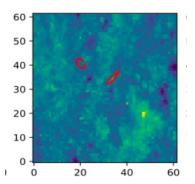
 <sup>[2]</sup> Chen, Wei, and Arun Ramamurthy. "Deep generative model for efficient 3D airfoil parameterization and generation." AIAA Scitech 2021 Forum. 2021.
 [3] Zhou, Linqi, Yilun Du, and Jiajun Wu. "3d shape generation and completion through point-voxel diffusion." Proceedings of the IEEE/CVF International Conference on Computer Vision. 2021.

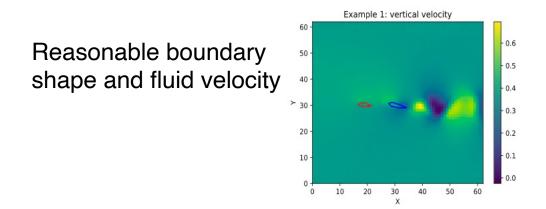
## Compositional inverse design: limitation of prior works

### 2. Recent methods using deep learning

- Limitations:
  - Easy to fall into adversarial mode

Designed boundary shape and fluid velocity





• Hard to design more complex parameters

Allen, Kelsey R., et al. "Physical design using differentiable learned simulators." *arXiv preprint arXiv:2202.00728* (2022).
 Chen, Wei, and Arun Ramamurthy. "Deep generative model for efficient 3D airfoil parameterization and generation." *AIAA Scitech 2021 Forum*. 2021.
 Zhou, Linqi, Yilun Du, and Jiajun Wu. "3d shape generation and completion through point-voxel diffusion." *Proceedings of the IEEE/CVF International Conference on Computer Vision*. 2021.

### Key components of our method

[1] **T. Wu\*,** T. Maruyama\*, L. Wei\*, T. Zhang\*, Y. Du\*, G. laccarino, J. Leskovec. "Compositional Generative Inverse Design." ICLR 2024 spotlight

- Simultaneously design the state U and the control/design variable  $\gamma$
- Joint objective with diffusion models

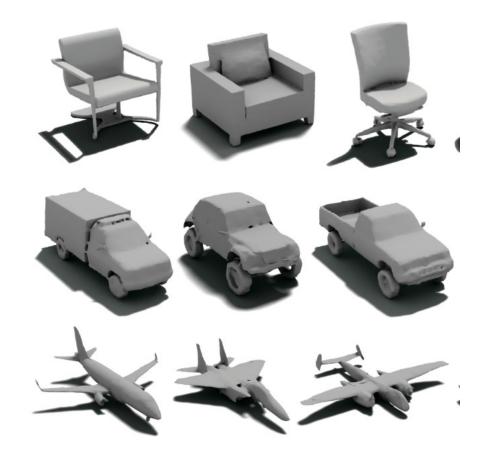
$$\hat{\gamma} = \operatorname*{arg\,min}_{\gamma, U_{[0,T]}} \left[ E_{\theta}(U_{[0,T]}, \gamma) + \lambda \cdot \mathcal{J}(U_{[0,T]}, \gamma) \right]$$

Compositional

## **Diffusion models**

Images and shapes generated by diffusion models:





#### By MeshDiffusion [1]

By DallE 2

## **Diffusion models**

#### Robotic policy by diffusion models [1]



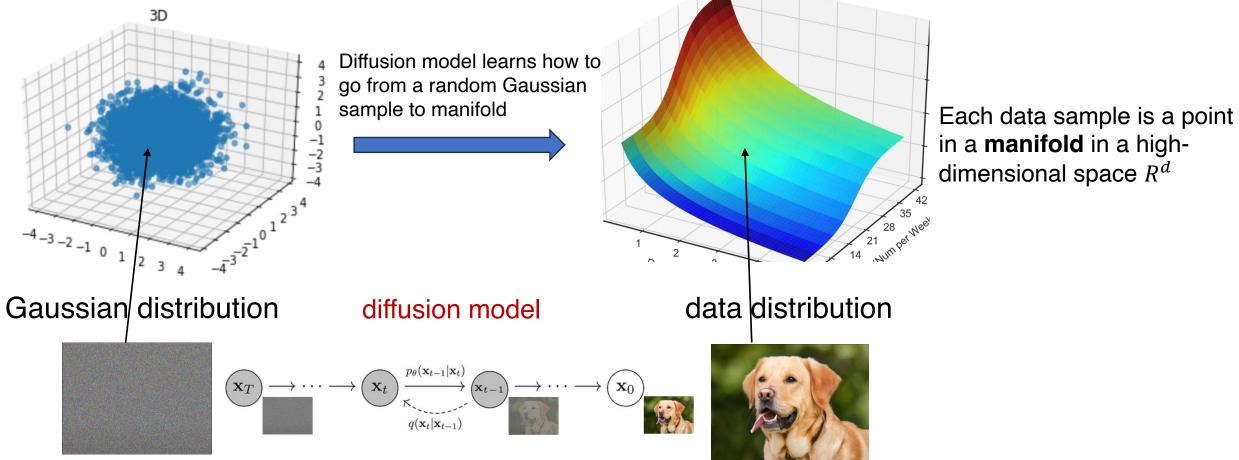
#### Text to video generation by Sora [2]



[1] Fu, Zipeng, Tony Z. Zhao, and Chelsea Finn. "Mobile ALOHA: Learning Bimanual Mobile Manipulation with Low-Cost Whole-Body Teleoperation." *arXiv preprint arXiv:2401.02117* (2024).
[2] OpenAI team. "Video generation models as world simulators", 2024

## **Diffusion models**

**Insight:** to construct a complex mapping from A to B, it is much easier to compose simple mappings



## DDPM: denoising diffusion probabilistic models [1]

 $x_0$ : training data  $x_t$ : training data with t steps of added noise Training:  $\epsilon_{\theta}$ : denoising network to be learned

Inference (sampling):

#### Algorithm 1 Training

1: repeat

- 2:  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
- 3:  $t \sim \text{Uniform}(\{1, \ldots, T\})$
- 4:  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- 5: Take gradient descent step on

 $\nabla_{\theta} \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta} (\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}, t) \right\|^2$ 

6: until converged

input: data with t steps of added noise predict: the noise  $\epsilon$  added

### Algorithm 2 Sampling

1:	$\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$	
2:	for $t = T,, 1$ do	,
	$\mathbf{z} \sim \mathcal{N}(0, \mathbf{I})$ if $t >$	
4:	$\mathbf{x}_{t-1} = rac{1}{\sqrt{lpha_t}} \left( \mathbf{x}_t + \mathbf{x}_t \right)$	$-\frac{1-lpha_t}{\sqrt{1-ar{lpha}_t}} \boldsymbol{\epsilon}_{ heta}(\mathbf{x}_t,t) \Big) + \sigma_t \mathbf{z}$
	end for	^
6:	return $\mathbf{x}_0$	denoise step-by-step

**Limitation:** Does not consider optimizing the samples with design objectives. Can only sample examples similar to the training distribution.

[1] Ho, Jonathan, Ajay Jain, and Pieter Abbeel. "Denoising diffusion probabilistic models." *Advances in neural information processing systems* 33 (2020): 6840-6851.

## Our method: intuition

x: data samples (e.g., image, trajectory)

Diffusion model essentially learns a "energy"-based model  $E_{\theta}$  to model the probability distribution  $p_{\theta}(x) \propto e^{-E_{\theta}(x)}$ 

The denoising function  $\epsilon_{\theta}(x_t)$  is essentially the gradient of the energy-based model

 $\epsilon_{\theta}(x) = \nabla_{x} E_{\theta}(x)$ 

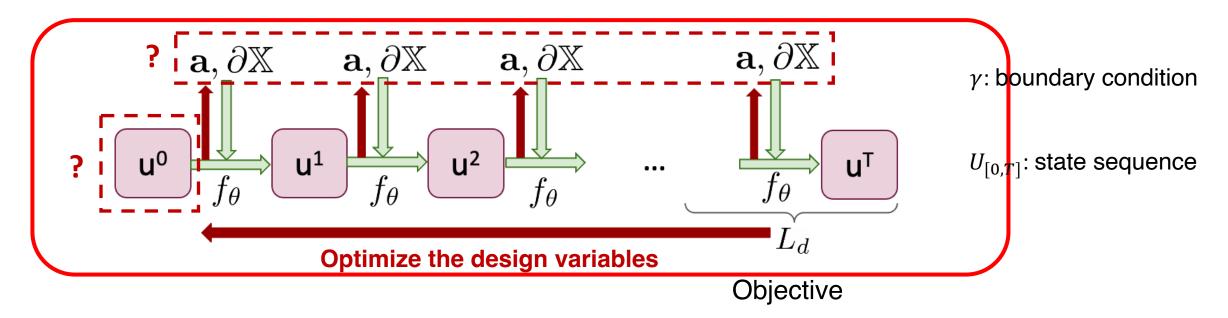
[1] **Wu, Tailin**, et al. "Compositional Generative Inverse Design." ICLR 2024 spotlight

$$\hat{\gamma} = \underset{\gamma, U_{[0,T]}}{\operatorname{arg\,min}} \left[ E_{\theta}(U_{[0,T]}, \gamma) + \lambda \cdot \mathcal{J}(U_{[0,T]}, \gamma) \right]$$
Training: only learn  $E_{\theta}$  Inference: have an additional objective  $\mathcal{J}$ 

decreasing J

 $U_{[0,T]}$ : state sequence  $\gamma$ : boundary condition

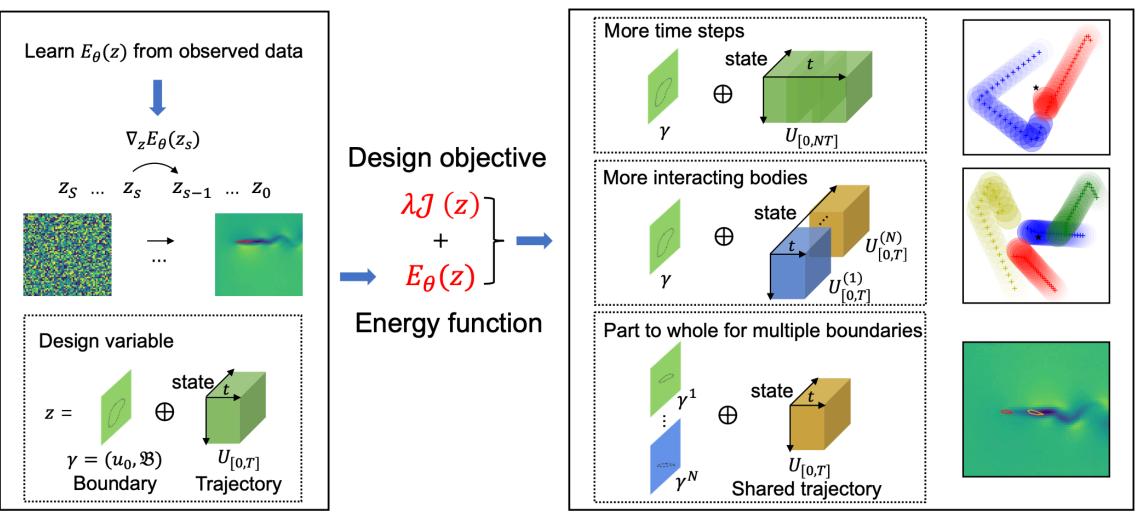
### Al for scientific design: definition



Treat all the variables as a single variable  $(U_{[0,T]}, \gamma)$  and learn to generate simultaneously

## Our method: architecture

Train



**Compositional Design** 

Fig.1 of CinDM. By composing generative models specified over subsets of inputs, we present an approach that design materials significantly more complex than those seen at training.

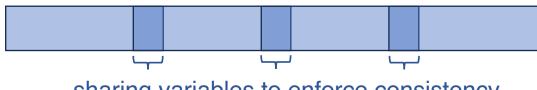
### Experiment 1: n-body simulation, time composition

**Train:** generate the simulation on 24 steps

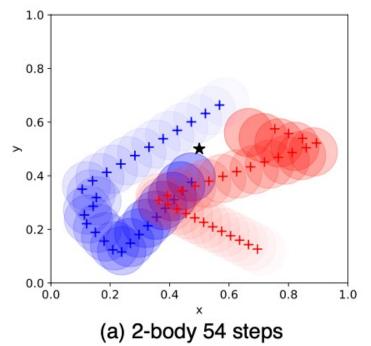


Inference: simulation on more time steps (e.g., 54 steps)

**Objective** *J***:** design the initial position and velocity of the two bodies such that their end position close to the center



sharing variables to enforce consistency



### Experiment 1: n-body simulation, time composition

	2-body 24 steps		2-body 34 steps		2-body 44 steps		2-body 54 steps	
Method	design obj	MAE						
CEM, GNS (1-step)	0.3021	0.14941	0.2531	0.13296	0.2781	0.20109	0.2845	0.19811
CEM, GNS	0.3144	0.12741	0.3178	0.16538	0.3102	0.24884	0.3059	0.24863
CEM, U-Net (1-step)	0.2733	0.08013	0.2680	0.13183	0.2910	0.14783	0.2919	0.13348
CEM, U-Net	0.2731	0.02995	0.2424	0.02937	0.2616	0.04460	0.2804	0.06520
Backprop, GNS (1-step)	0.1216	0.03678	0.1643	0.02976	0.1966	0.03645	0.2657	0.10331
Backprop, GNS	0.2453	0.13024	0.2822	0.11200	0.2959	0.12867	0.2877	0.14241
Backprop, U-Net (1-step)	0.2020	0.06338	0.2193	0.07705	0.2187	0.05668	0.2851	0.07716
Backprop, U-Net	0.1168	0.01137	0.1294	0.01303	0.1481	0.00804	0.3140	0.01675
CinDM (ours)	0.1143	0.01202	0.1251	0.00763	0.1326	0.00695	0.1533	0.00870

Our method (CinDM) achieves the *best* design objective with (mostly) *lowest* simulation MAE

Baselines: Backpropagation through time [1] and cross-entropy method (CEM) [2]

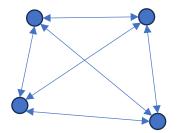
[1] Allen, Kelsey R., et al. "Physical design using differentiable learned simulators." *NeurIPS* 2022
[2] Reuven Y Rubinstein and Dirk P Kroese. The cross-entropy method: a unified approach to combinatorial optimization, Monte-Carlo simulation, and machine learning, volume 133. Springer, 2004.

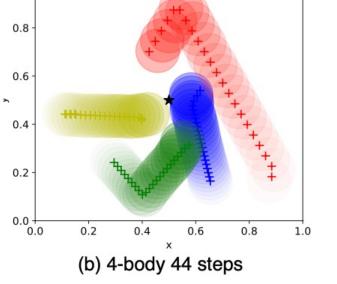
### Experiment 2: n-body simulation, state composition

Train: generate the simulation on 2 bodies

Inference: simulation on more bodies (e.g., 4 or 8 bodies)

**Objective** J: design the initial position and velocity of the n bodies such that their end position close to the center





1.0

treat the n-body interaction as composition of multiple 2-body interactions

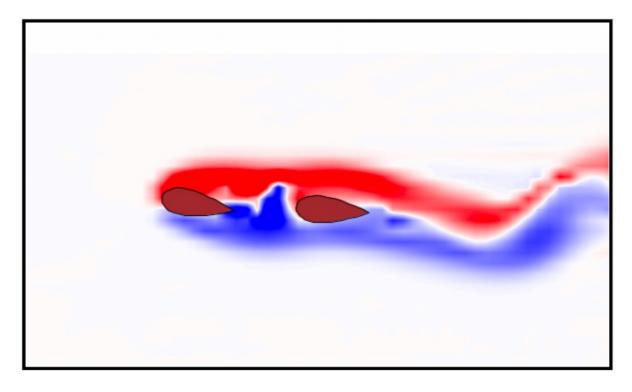
### Experiment 2: n-body simulation, state composition

	4-body 24 steps		4-body 44 steps		8-body 24 steps		8-body 44 steps	
Method	design obj	MAE						
CEM, GNS (1-step)	0.3029	0.20027	0.3215	0.26518	0.3312	0.36865	0.3292	0.37430
CEM, GNS	0.3139	0.21253	0.3110	0.26924	0.3221	0.26708	0.3319	0.32678
Backprop, GNS (1-step)	0.2872	0.08023	0.2900	0.11331	0.3312	0.27988	0.3227	0.74314
Backprop, GNS	0.3118	0.10249	0.3423	0.15277	0.3302	0.19039	0.3233	0.24718
CinDM (ours)	0.2066	0.04152	0.2281	0.03195	0.3056	0.08821	0.3169	0.09566

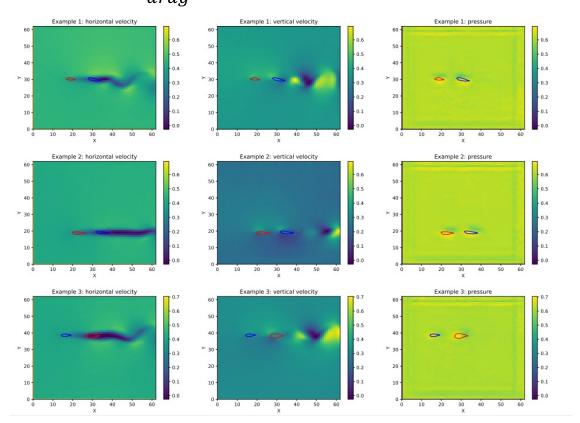
Our method (CinDM) achieves the best design objective with lowest simulation MAE

Training: consider a single airfoil interacting with the air flow

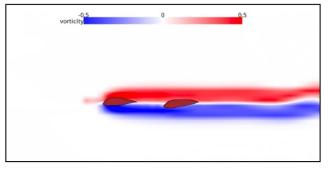
**Inference:** consider **multiple airfoils**, maximize life-to-drag ratio:  $(=\frac{lift}{drag})$ 



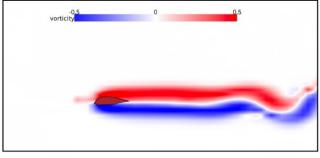
Example of Lily-Pad simulation



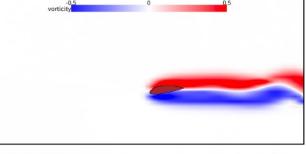
**Compositional design results** of our method in 2D airfoil generation. Each row represents an example. We show the heatmap of velocity in horizontal and vertical direction and pressure in the initial time step, <sub>24</sub> inside which we plot the generated airfoil boundaries.



(a) Formation flying of airfoils A and B



(b) Single flying of airfoil A

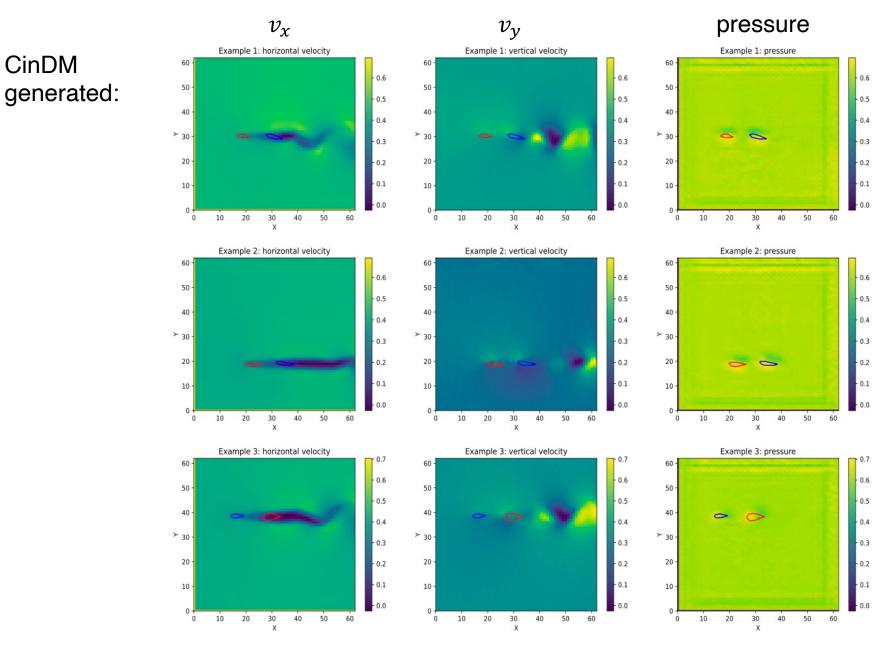


(c) Single flying of airfoil B

#### Our model discovers formation flying

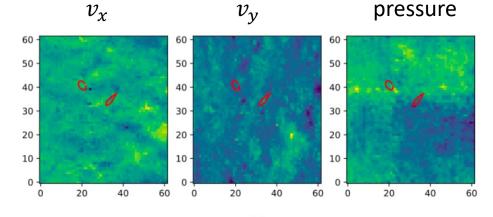
- Reducing the drag by 53.6%
- increasing the lift-to-drag ratio by 66.1%

	1	airfoil	2 airfoils		
Method	design obj↓	lift-to-drag ratio ↑	∣ design obj↓	lift-to-drag ratio ↑	
CEM, FNO CEM, LE-PDE	0.0932 0.0794	1.4005 1.4340	0.3890 0.1691	1.0914 1.0568	
Backprop, FNO Backprop, LE-PDE	<b>0.0281</b> 0.1072	1.3300 1.3203	0.1837 0.0891	0.9722 0.9866	
CinDM (ours)	0.0797	2.177	0.1986	1.4216	

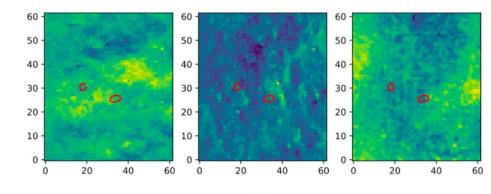


### Experiment 3: inverse design by baseline neural models

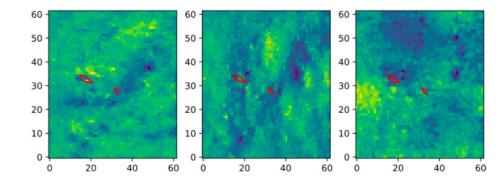
Adversarial modes by baseline neural model (FNO with CEM):







(b)



## Summary

#### **Compositional inverse design:**

• Design boundaries and states more complex than in training

### Our CinDM method:

$$\hat{\gamma} = \operatorname*{arg\,min}_{\gamma, U_{[0,T]}} \left[ E_{\theta}(U_{[0,T]}, \gamma) + \lambda \cdot \mathcal{J}(U_{[0,T]}, \gamma) \right]$$

- View inverse design problem as energy minimization on the learned energy function and design objective, on the joint variable of state and boundary.
- Composition by adding energy functions
- Achieves state-of-the-art performance on n-body and airfoil design

Welcome collaborations and tackle important problems together! Contact: <u>wutailin@westlake.edu.cn</u>. Homepage: <u>http://tailin.org</u>









#### My group's research interest:

- Al for accelerating scientific simulation, design, and control
- Al for scientific discovery

Contact: <a href="mailto:wutailin@westlake.edu.cn">wutailin@westlake.edu.cn</a>. Homepage: <a href="http://tailin.org">http://tailin.org</a>



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