Compositional Generative Inverse Design

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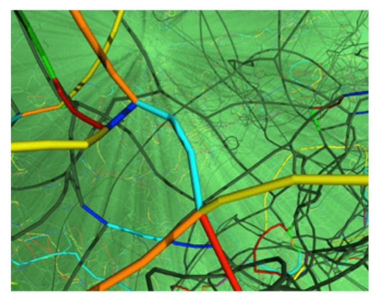
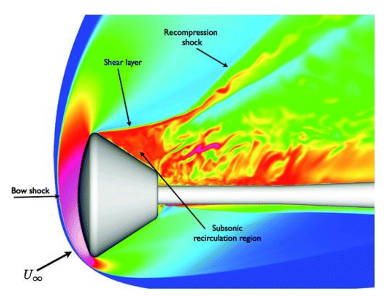
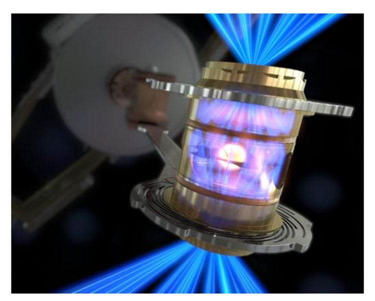
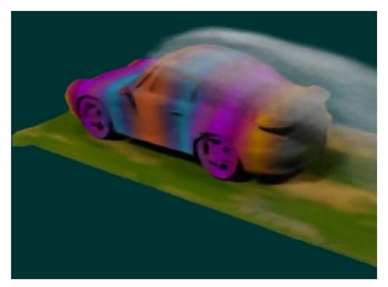
Motivation

- Inverse design is an important task to find a set of high-dimensional design parameters for a dynamical system to optimize an objective under a set of constraints. It has wide applications in both science and engineering.
- Compositional inverse design is an inverse design task that finds a set of optimal parameters for a dynamical system that contains more parameters than seen datasets.


Materials science


Mechanical engineering


Controlled nuclear fusion


Equipment manufacturing

Key challenges:

- Complex design space and high computational cost
- How to characterize the complex dynamics and interactions among components within a physical process?
- How to generalize to more complex composition scenarios?

- Traditional physical simulation methods

Pros: (1) first principle-based, (2) accurate, (3) error guaranteed.
Challenges: (1) high computational cost, (2) requirements for rich expert knowledge, (3) weak at dealing with high-dimensional design space

- Recent deep learning-based methods

Pros: (1) alleviates much engineering efforts. (2) Offer speedup
Challenges: (1) still need huge computation via system evolution, (2) easy to fall into adversarial mode, (3) hard to generalize to more complex composition scenarios beyond training set

- Summary of prior works:

Existing methods have significant limitations such as easily getting stuck in suboptimal solutions and inability to generalize.

QR code for paper

Approach

Problem setting:

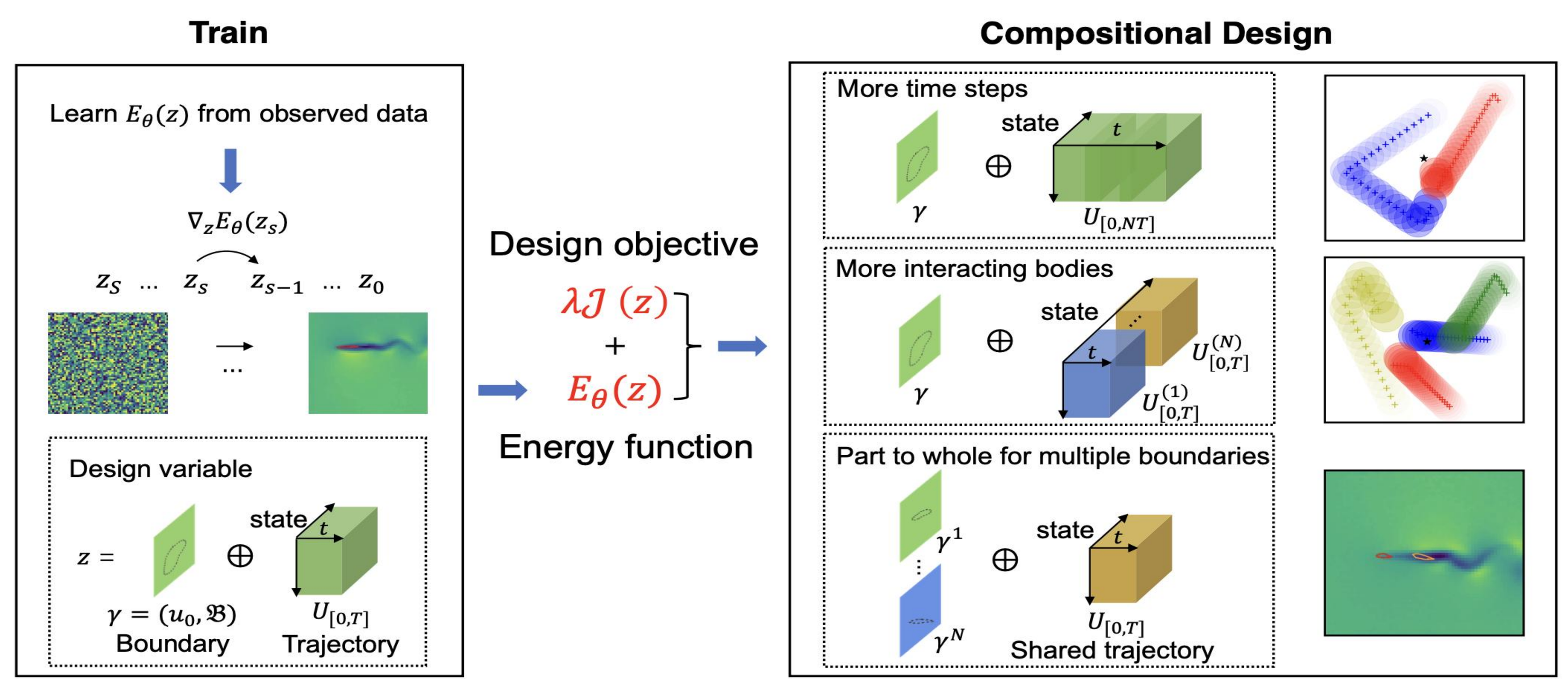
- Simultaneously design the state U and the parameter γ (e.g., boundary and initial conditions).
- Joint objective:

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

E_θ: energy-based model; serves the purpose of a surrogate model in approximating simulator dynamics
$\mathcal{J}$: design objective

Keypoints of CinDM:

- Uses energy functions to implicitly govern dynamics and interactions among different components faithfully in the system
- Uses diffusion model to learn the energy functions of composition
- Introduces the design objective effectively during inference, while ensuring physical consistency



Implementation of CinDM

- Training: $L_{MSE} = \left\| \epsilon - \epsilon_\theta\left(\sqrt{1-\beta_s}\, z + \sqrt{\beta_s}\, \epsilon, s\right) \right\|_2^2, \ \epsilon \sim N(0, I)$
- Compositional inference:

$$z_{s-1} = z_s - \eta \frac{1}{N} \sum_{i=1}^{N} \left(\epsilon_\theta^i(z_s^i, s) + \lambda \nabla_z \mathcal{J}(z_s) \right) + \xi, \quad \xi \sim \mathcal{N}(0, \sigma_s^2 I)$$

- 1. Generalization to more time steps

$$E_\theta(U_{[0,T]}, \gamma) = \sum_{i=1}^{N} E_\theta\left(U_{[(i-1)\cdot t_q, i\cdot t_q + T^{tr}]}, \gamma\right)$$

- 2. Generalization to more interacting bodies

$$E_\theta(U_{[0,T]}, \gamma) = \sum_{i<j} E_\theta(U^{(i)}_{[0,T]}, U^{(j)}_{[0,T]}, \gamma)$$

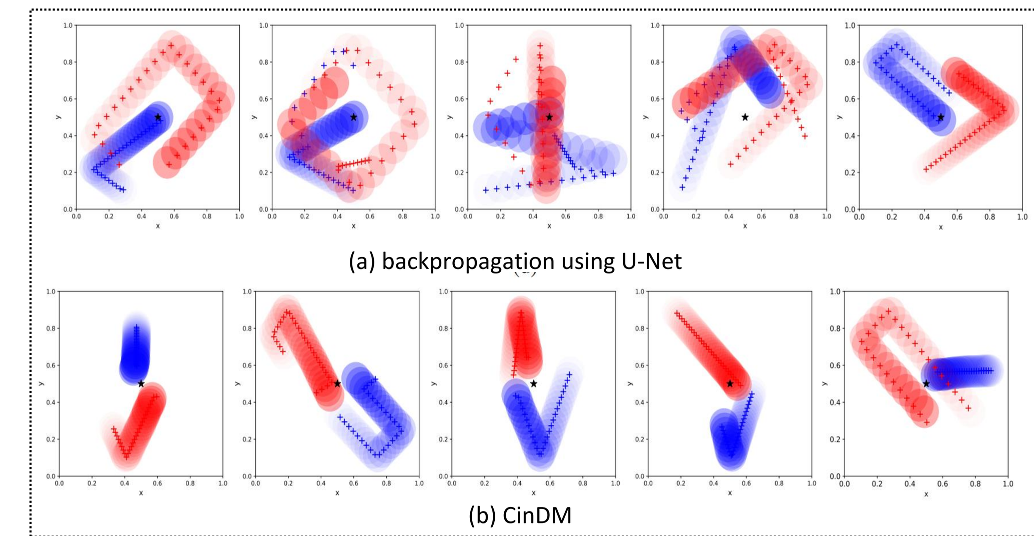
- 3. Generalization from part to whole for boundaries.

$$E_\theta(U_{[0,T]}, \gamma) = \sum_{i=1}^{N} E_{\theta_i}(U_{[0,T]}, \gamma^i)$$

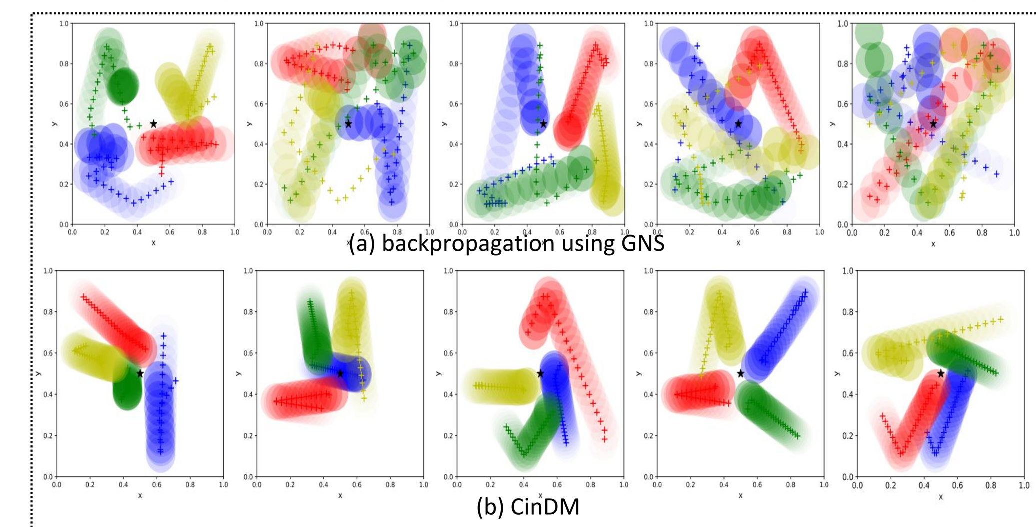
Results

- Our method outperforms state-of-the-art neural inverse design method by an average of 41.5% in prediction MAE and 14.3% in design objective for the N-body dataset
- Our method discovers formation flying to minimize drag in the multi-airfoil design task.

N-body task

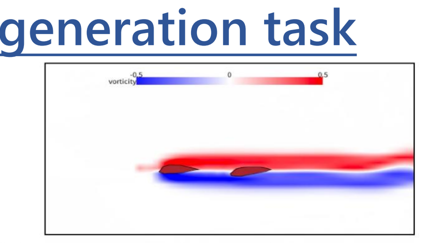

(a) backpropagation using U-Net
(b) CinDM

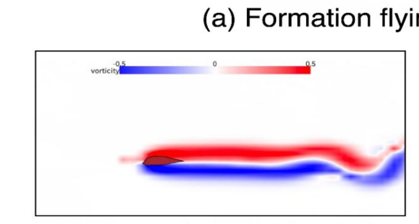
Compositional inverse design in time: 2-body 54 steps: results of the best baseline(backpropagation using U-Net) and CinDM

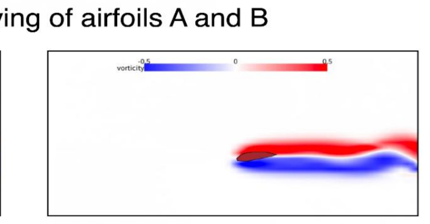

(a) backpropagation using GNS
(b) CinDM

Compositional inverse design generalizing to more objects: 4-body 44 steps: results of the best baseline (backpropagation using GNS) and CinDM

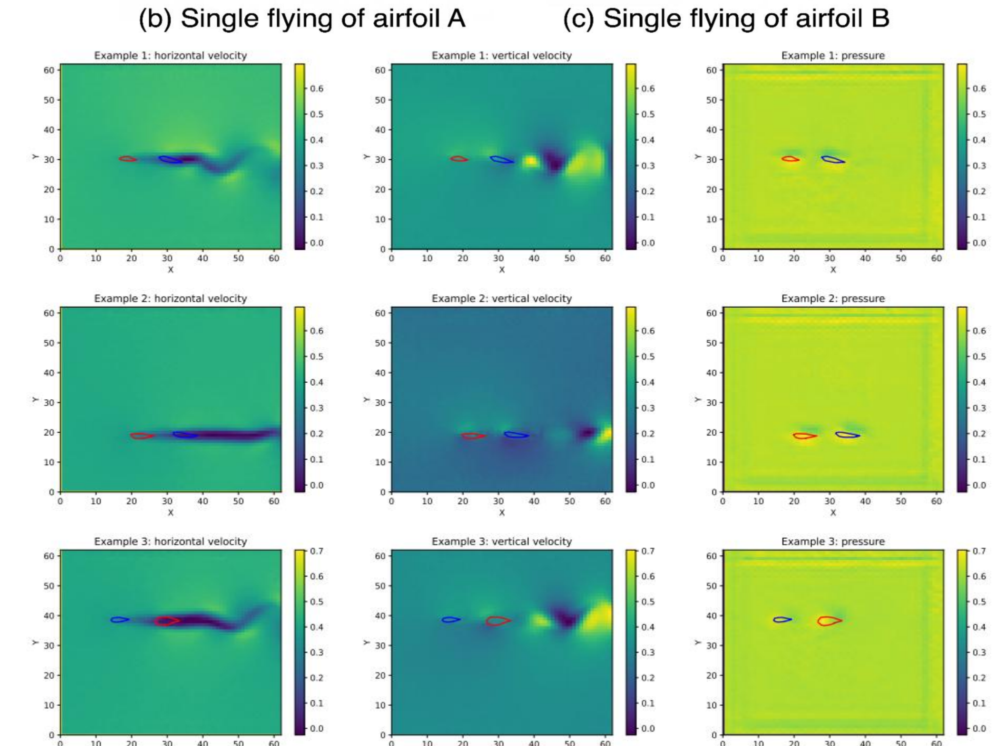
2D airfoils generation task


(a) Formation flying of airfoils A and B


(b) Single flying of airfoil A


(c) Single flying of airfoil B

Discovered formation flying. Our model's designed boundary forms a "leader'' and "follower" formation (a), reducing the drag by 53.6% and increasing the lift-to-drag ratio by 66.1% compared to each airfoil flying separately (b)(c).



Compositional design results of our method in 2D airfoil generation. Each row represents an example. We show velocities in horizontal and vertical directions and pressure in the initial time step, inside which we plot the generated airfoil boundaries.