Parametric model reduction of mean-field and stochastic systems via higher-order action matching

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Overview

We learn models of population dynamics of physical systems that feature stochastic and mean-field effects and that depend on physics parameters.

- Building on the Benamou-Brenier formula and action matching [2], we infer population dynamics from a **simulation-free variational objective**.
- The inferred gradient fields can then be used to **predict the populations dynamics for unseen physics parameters**.
- Higher-order quadrature is **critical for accurately estimating the training objective**.
- HOAM yields **orders of magnitude speed-up** compared to classical numerical models.

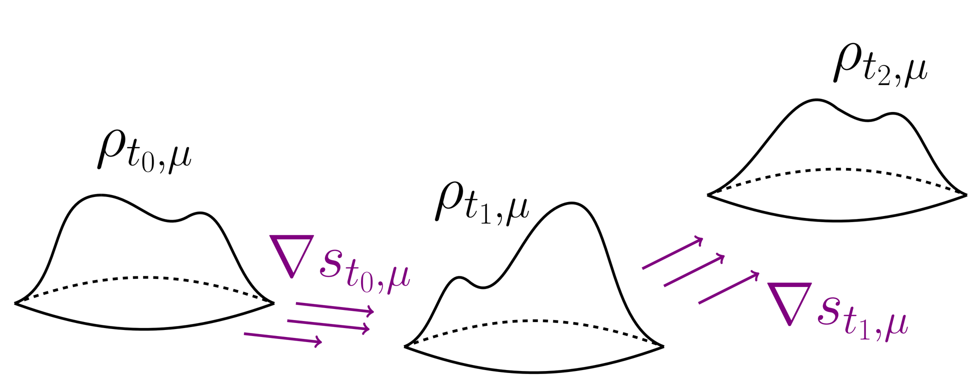
Parameter-dependent population dynamics

Population dynamics of $X_{t,\mu} \sim \rho_{t,\mu}$ can be described by the continuity equation

$$\partial_t \rho_{t,\mu} = -\nabla \cdot (\rho_{t,\mu} \nabla s_{t,\mu}), \qquad \text{for all } t \in [0,1], \mu \in \mathcal{D}, \tag{1}$$

with the initial condition $\rho_{t=0,\mu} =: \rho_{0,\mu}$ and gradient vector field $\nabla s_{t,\mu}$.

In our case the continuity equation (1) depends on the physics parameter $\mu \sim \nu$.



Higher-order quadrature for estimating the loss

The continuous variational form of (1) reads

$$E(s) := \mathbb{E}_{\mu\sim\nu}\left[\int_0^1 \mathbb{E}_{x\sim\rho_{t,\mu}}\left[\frac{1}{2}|\nabla s_{t,\mu}|^2 + \partial_t s_{t,\mu}\right] - \mathbb{E}_{x\sim\rho_{t,\mu}}\left[s_{t,\mu}\right]\Big|_{t=0}^{t=1}\right]. \tag{2}$$

We discretize this using a combination of Monte-Carlo and higher-order quadrature:

$$\hat{E}(s) := \hat{\mathbb{E}}^{n_\mu}_{\mu\sim\nu}\left[\sum_{n=1}^{n_t} w_n \hat{\mathbb{E}}^{n_x}_{x\sim\rho_{t_n,\mu}}\left[\frac{1}{2}|\nabla s_{t_n,\mu}|^2 + \partial_t s_{t_n,\mu}\right] - \hat{\mathbb{E}}^{n_x}_{x\sim\rho_{t,\mu}}\left[s_{t,\mu}\right]\Big|_{t=0}^{t=1}\right] \tag{3}$$

where w_n are numerical quadrature weights and t_n are the corresponding nodes.

After training, new samples can be generated by integrating

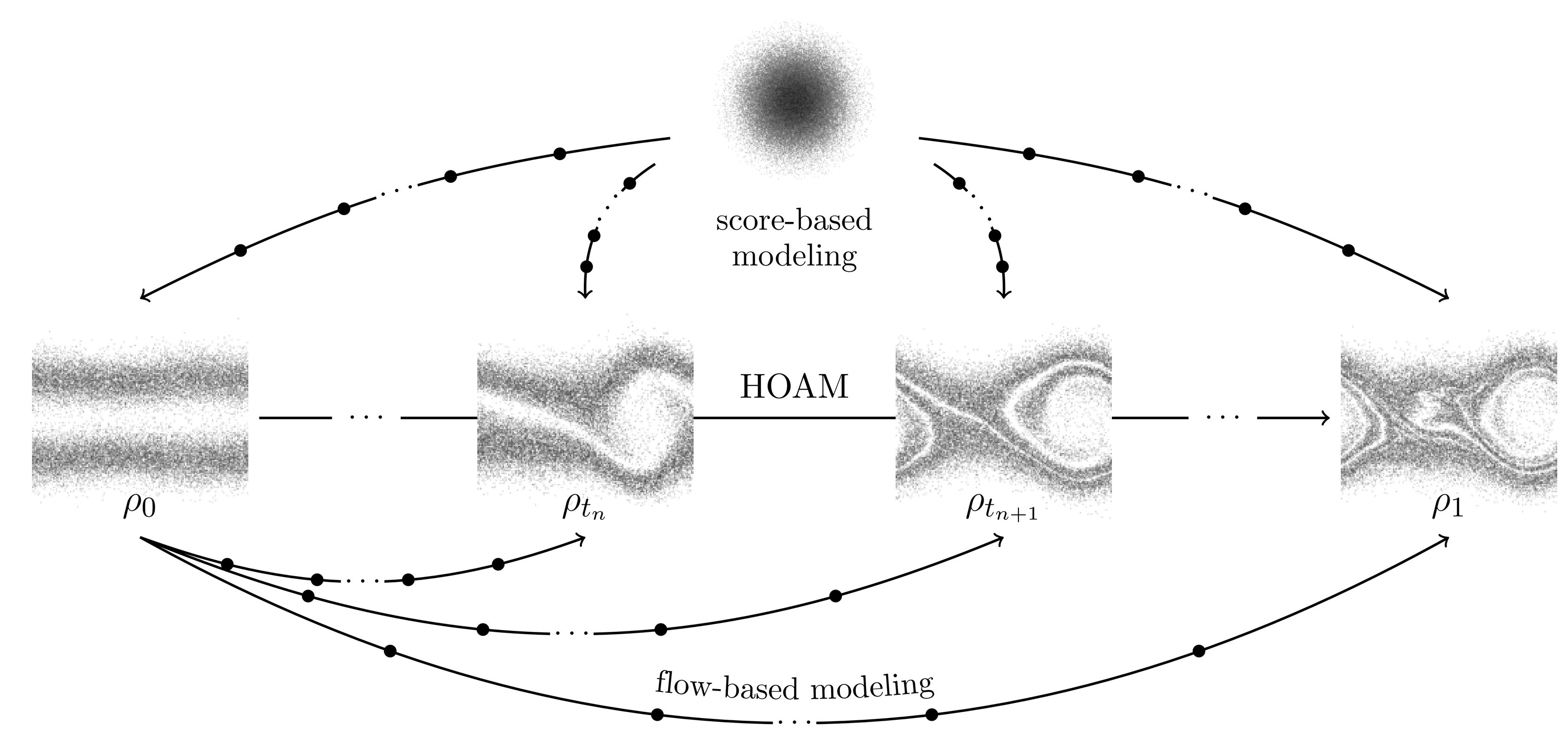
$$\frac{\mathrm{d}}{\mathrm{d}t} X_{t,\mu} = \nabla s_{t,\mu}(X_{t,\mu}), \quad X_{0,\mu} \sim \rho_{0,\mu}. \tag{4}$$

We show that the numerical quadrature in HOAM is critical for accurately estimating the training objective from sample data and for stabilizing the training process.

1 J. Berman*, T. Blickhan*, B. Peherstorfer, *Parametric model reduction of mean-field and stochastic systems via higher-order action matching*. NeurIPS 2024.

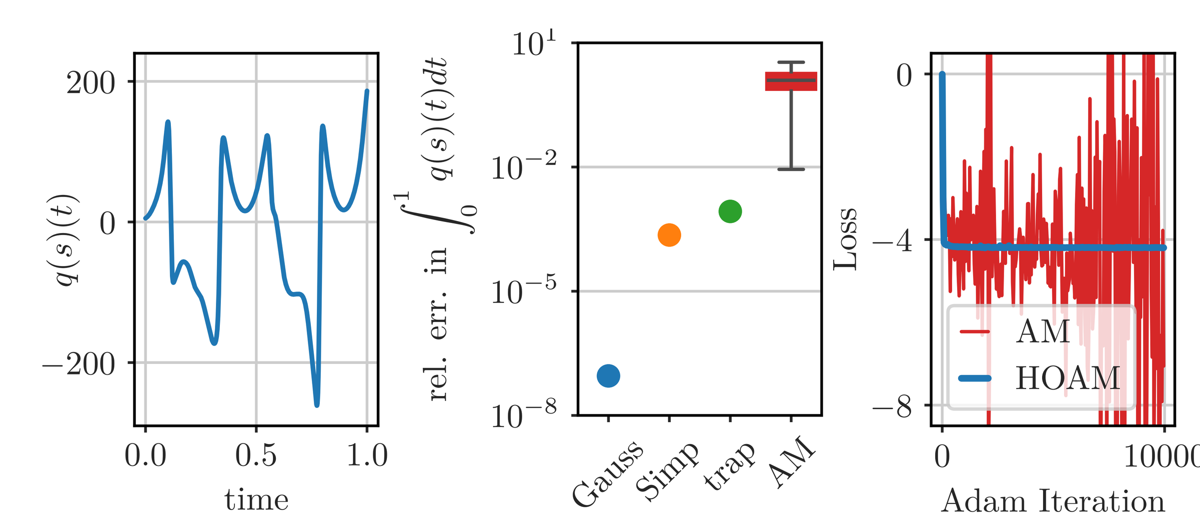
2 K. Neklyudov, R. Brekelmans, D. Severo, A. Makhzani, *Action Matching: Learning Stochastic Dynamics from Samples*. ICML 2023.

Rapid predictions (inference) with learned reduced models



In HOAM, time t in the SDE used for generating samples is the same time as of the physics problem, thus the costs of inference scales with the trajectory length.

HOAM stabilizes training with higher-order quadrature



- **Left**: To evaluate (3), $q(s)(t) = \hat{\mathbb{E}}^{n_x}_{x\sim\rho_t}\left[\frac{1}{2}|\nabla s_t|^2 + \partial_t s_t\right]$ is numerically integrated.
- **Center**: Numerical quadrature gives accurate estimates of the time integral.
- **Right**: Numerical quadrature in HOAM leads to stable estimates of the loss.

Challenging loss estimation

- The loss (2) only defines s up to an additive constant that can change in time. If $t \mapsto s(t)$ minimizes (2), then so does $t \mapsto s(t) + f(t)$ for any $f : [0,1] \mapsto \mathbb{R}$:

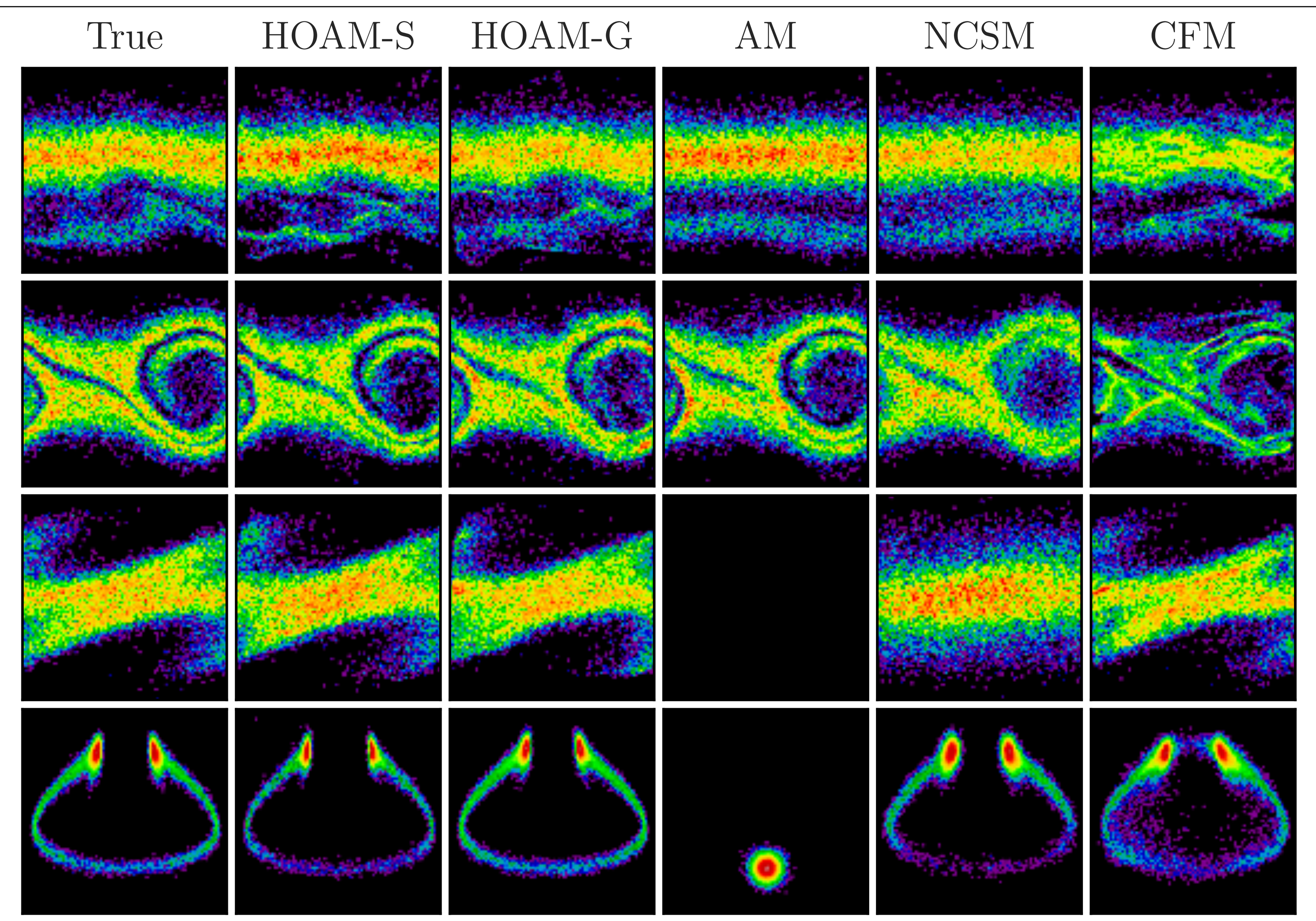
$$E(s+f) - E(s) = \int_0^1 \partial_t f(t)\,\mathrm{d}t - f(1) + f(0) = 0. \tag{5}$$

- Discretely, the difference depends on the quadrature error:

$$\hat{E}(s+f) - \hat{E}(s) = \sum_n w_n \partial_t f(t_n) - f(1) + f(0) \neq 0. \tag{6}$$

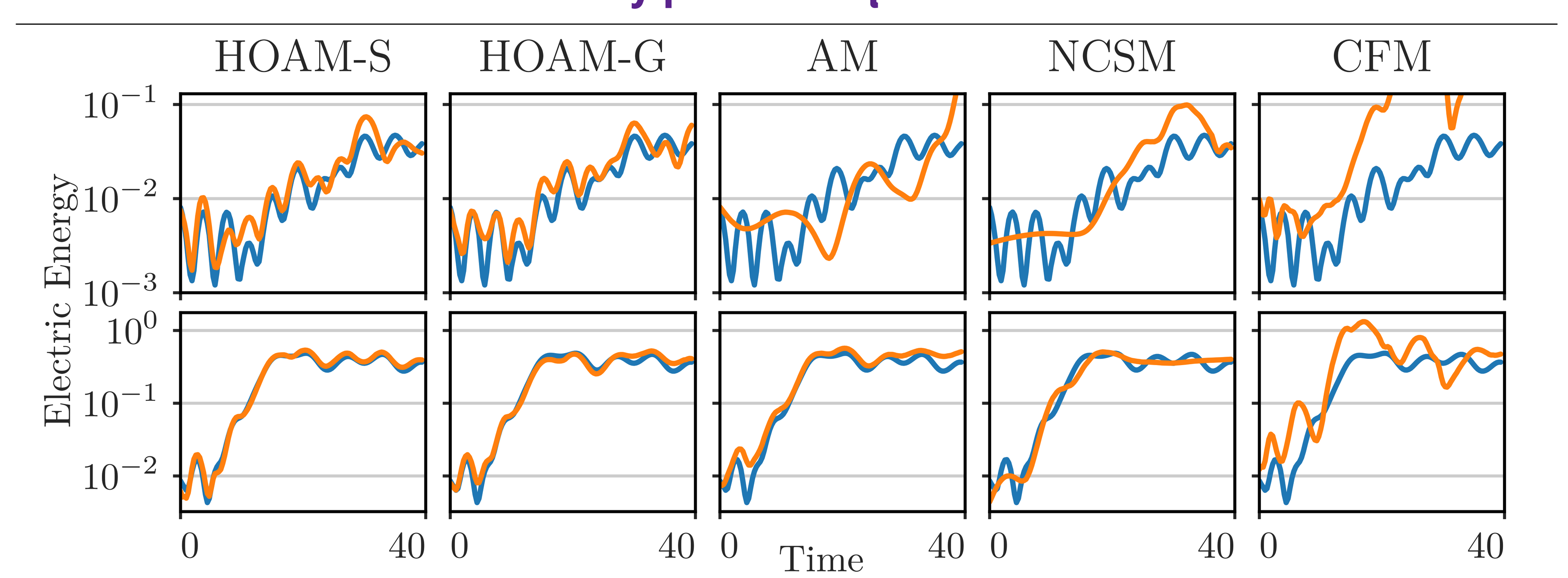
- **During optimization, f and $\partial_t f$ can grow to the point where the training becomes unstable as soon as the quadrature error term is too large.**

HOAM compared to time-conditioned flow-based models



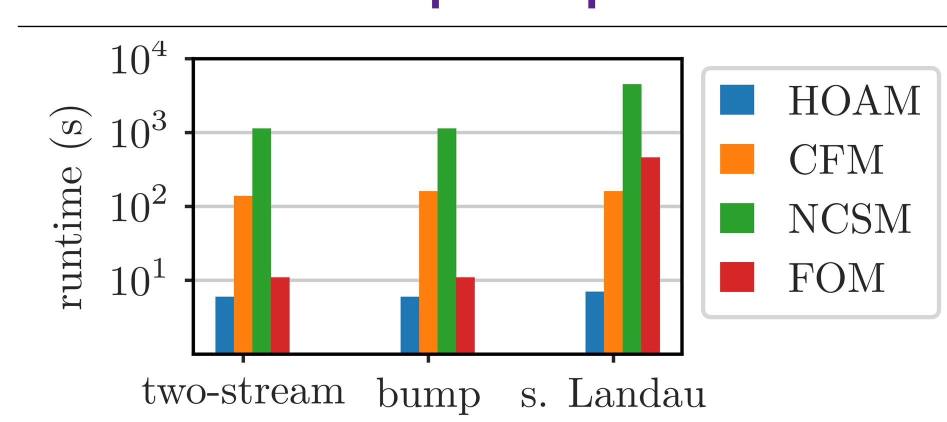
- **Top**: Bump-on-tail ($t = 20$) instability. **Middle top**: two-stream ($t = 20$) instability. **Middle bottom**: Strong Landau damping ($t = 4$). **Bottom**: Nine-dimensional chaos.

HOAM accurately predicts quantities of interest



HOAM accurately predicts the energy growth in the transient regime and oscillations at later times. The competing flow-based methods are less accurate.

Speedups in inference step (predictions)



- HOAM provides about 2 orders of magnitude speedup over the 6D full-order particle-in-cell model.
- Other surrogate models provide no speedup.

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