

Weekly Progress Report, Feb 27 2026

Literature Review

This week I read the Kevrekidis paper and the Reiss paper:

1. **Sonday, Singer & Kevrekidis (2011)**, arXiv:1104.0725. They build a Hermitian matrix from pairwise snapshot alignments and extract optimal shifts from its leading eigenvectors, then combine symmetry quotienting with dimensionality reduction via vector diffusion maps.
2. **Reiss, Schulze, Sesterhenn & Mehrmann (2018)**, arXiv:1512.01985. They formally define sPOD for multiple transport velocities, introducing time-dependent shifts per transport component and optimizing them jointly via an iterative procedure.

Takeaway: Our approach is simpler: single reference field (temporal mean), FFT cross-correlation, one-shot, no iterative optimization. Works because our system has one dominant transport mode.

What Our sPOD Does

We convert particles on a periodic 2D box into 64×64 KDE density images. The flock translates, so standard POD wastes modes on position. We shift every frame to a common location via FFT cross-correlation against the temporal mean, using `numpy.roll` (exact, no interpolation). After quotienting out translation, POD only represents shape dynamics, and the singular values decay much faster.

Experiments and Results

I ran DYN1–DYN6 covering: gentle Vicsek, hypervelocity, high noise, strong attraction, log/sqrt density transforms, and variable speed. I also ran an ablation suite (XABL1–XABL8) as a 2^3 factorial over {transform, simplex, spectral scaling}, all with alignment on. Reconstruction R^2 from the DYN suite (all MVAR, all with sPOD): DYN3 (high noise) 0.98, DYN4 (strong attraction) 0.95, DYN2 (hypervelocity) 0.91, DYN6 (variable speed) 0.89, DYN1 (gentle baseline) 0.81. 1-step teacher-forced R^2 was 0.93–0.98 across all, and the POD ceiling exceeded 0.99.

Main findings:

- **Alignment dominates.** $\sqrt{\rho} +$ simplex help 1–3% in R^2 but become negligible once shift alignment is on. Alignment alone raises R^2 from ~ 0.5 –0.7 to $\sim 0.95+$.
- **R^2 degrades over time** depending on regime. Clustering regimes maintain high R^2 past 200s; after sPOD the quotient-space dynamics are nearly Markovian.
- **Strong repulsion** (no attraction): lower performance because shape dynamics are more complex.
- **Singular value decay:** $d = 19$ captures $>99.9\%$ of variance with sPOD vs. $\sim 96\%$ without.

LSTM Fix and Regime Testing

I fixed the LSTM training code: wrong config keys (`hidden_size` → `hidden_units`, `epochs` → `max_epochs`) and missing parameters (dropout, gradient clipping, layer norm). The LSTM now runs across all regimes. Both LSTM and MVAR produce comparable results in clustering regimes.

Proposed Next Steps

1. **Systematic MVAR vs. LSTM comparison.** Run both models across DYN1–6 plus milling, double mill, swarming, and escape (regimes from the Bhaskar topology paper and the d’Orsogna model) under identical conditions (same horizon, POD threshold, training size, particle count, hyperparameters).
2. **Per-regime analysis.** For each regime: POD vs. sPOD eigenvalue decay, forecast R^2 over time (MVAR vs. LSTM), true vs. predicted density snapshots, and order parameter tracking.
3. **Thesis figures.** Combine SVD decay and phase dynamics with empirical results across all regimes.
4. **If time allows, alternative sPOD methods.** (a) Kevrekidis eigenvalue alignment via the Hermitian pairwise-connection matrix. (b) Reiss et al. multi-frame sPOD for multiple clusters.
5. **WSINDy.** Fit WSINDy to all regimes and compare.

Figures

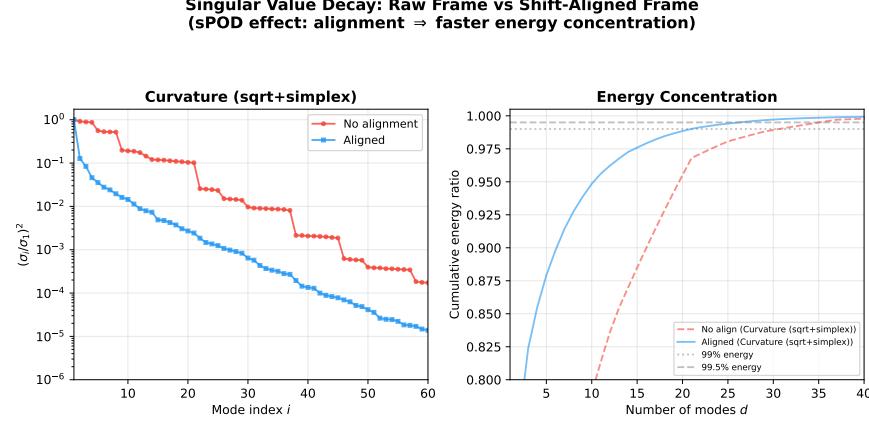


Figure 1: Singular value decay: standard POD vs. sPOD. With sPOD, 19 modes capture $>99.9\%$ of energy.

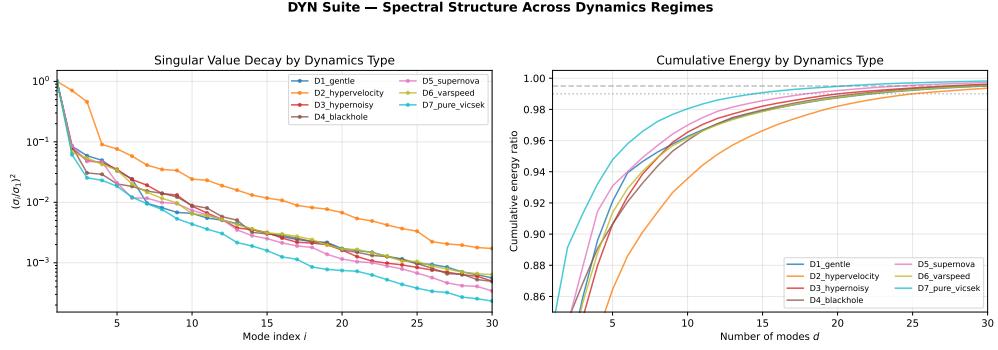


Figure 2: sPOD singular value spectra across the DYN suite. Spectral knee at modes 3–5 for most regimes; DYN6 (variable speed) decays slower.

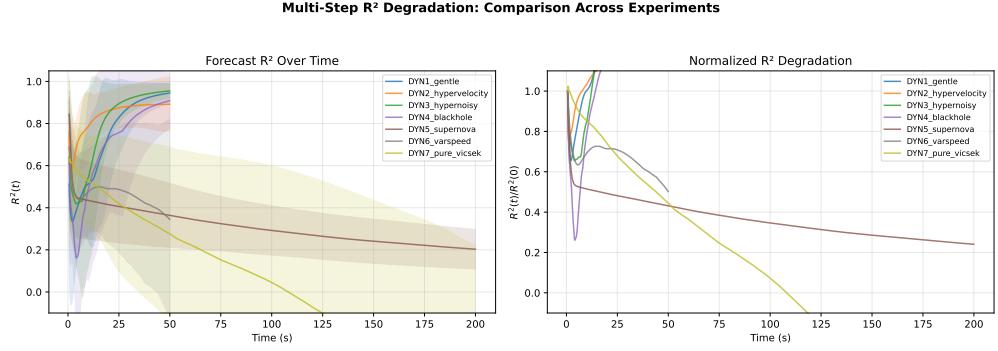
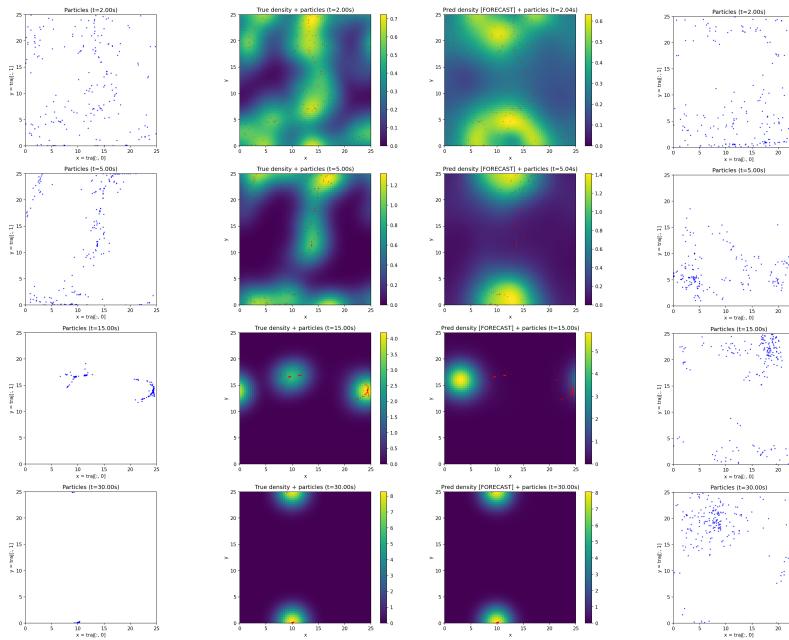


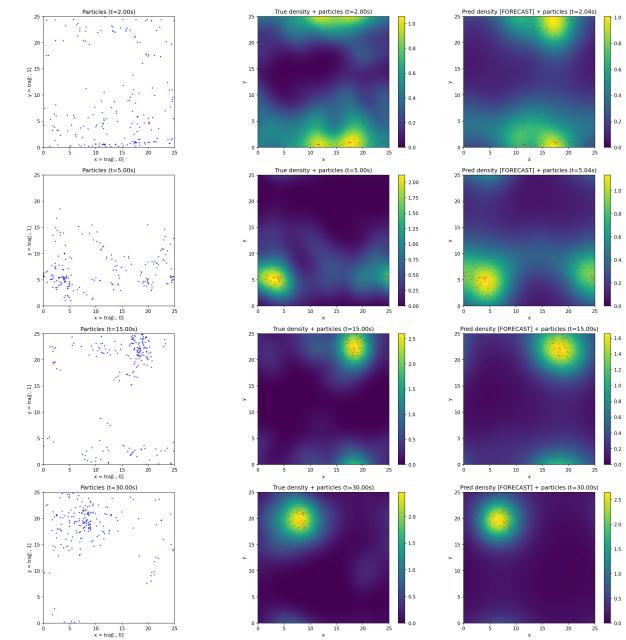
Figure 3: Forecast R² vs. prediction horizon. I tested each regime at different horizons; the final pipeline will use the same horizon for all. Clustering regimes stay high past 100s; non-clustering regimes degrade faster.

DYN1_gentle_v2 test_000 — KDE == Trajectory Alignment Check
Red dots = particle positions. They should overlap density peaks.



(a) DYN1 (gentle Vicsek)

DYN6_varspeed_v2 test_000 — KDE == Trajectory Alignment Check
Red dots = particle positions. They should overlap density peaks.



(b) DYN6 (variable speed)

Figure 4: KDE alignment check. Left column: raw density. Right column: after shift alignment.

Phase Dynamics Analysis: Shift $\Delta(t)$ as Separate Dynamical Variable (sPOD / Moving-Frame Decomposition)

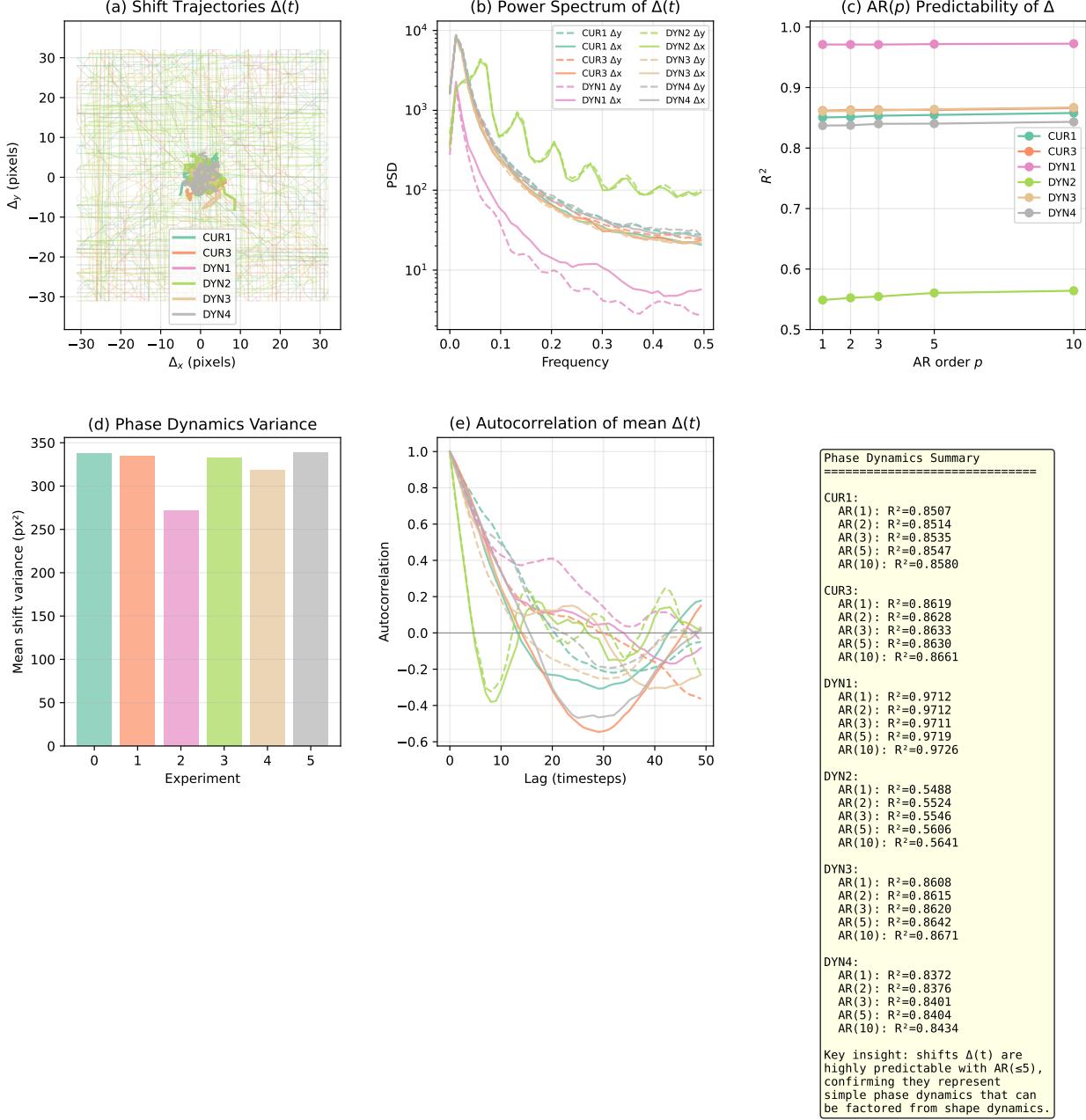


Figure 5: Phase dynamics of the shift sequence $\Delta(t)$. (a) Shift trajectories. (b) PSD: energy concentrated at low frequencies. (c) AR(p) predictability: AR(1) $R^2 > 0.95$, AR(5) ~ 0.999 . (d) Phase variance across experiments. (e) Autocorrelation: slow decay confirms persistence.