Quantum Mechanical Closure of Partial Differential Equations with Symmetries

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Statistical and Computational Challenges
in Probabilistic Scientific Machine Learning
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Motivation

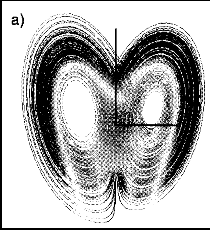
Original system

$$x_{n+1} = \Phi(x_n, \xi(y_n))$$
$$y_{n+1} = \Psi(x_n, y_n)$$

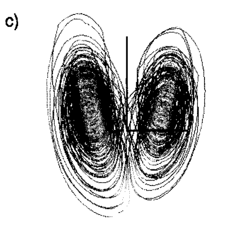
Parameterized system

$$x_{n+1} = \tilde{\Phi}(x_n, \tilde{\xi}(\tilde{y}_n))$$
$$\tilde{y}_{n+1} = \tilde{\Psi}(x_n, \tilde{y}_n)$$

Lorenz 63



Stochastic closure



[Palmer 01]

Dirac–von Neumann axioms of quantum mechanics

1. States are density operators, i.e., positive, trace-class operators $\rho\colon H \to H$ on a Hilbert space H, with $\operatorname{tr}\rho = 1$.

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2. (Bounded) observables are self-adjoint operators, $A\colon H \to H$.

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2. (Bounded) observables are self-adjoint operators, $A\colon H \to H$.
3. Measurement expectation and probability:

$$\mathbb{E}_\rho A = \operatorname{tr}(\rho A), \quad \mathbb{P}_\rho(\Omega) = \mathbb{E}_\rho(E(\Omega)), \quad A = \int_{\mathbb{R}} a \, dE(a).$$

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4. State evolution between measurements:

$$\rho_t = U^{t*} \rho_0 U^t.$$

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5. State conditioning by measurement (quantum Bayes' rule):

$$\rho|_e = \frac{\sqrt{e}\rho\sqrt{e}}{\operatorname{tr}(\sqrt{e}\rho\sqrt{e})}, \quad 0 < e \le I.$$

Embedding dynamics into a quantum mechanical system

[G. 19; Freeman et al. 23]

Probability densities $\mathcal{P}(\mu) \xrightarrow{P} \mathcal{P}(\mu)$

- $T: X \to X$: Dynamical flow with invariant measure μ.
- $\mathcal{P}(\mu)$: Probability densities in $L^1(\mu)$.
- $P: \mathcal{P}(\mu) \to P(\mu)$: Transfer operator, $P\nu = \nu \circ T^{-t}$.
- $L^\infty(\mu)$: Algebra of classical observables.
- $U: H \to H$: Unitary Koopman operator on $H = L^2(\mu)$, $Uf = f \circ T$.

Embedding dynamics into a quantum mechanical system

[G. 19; Freeman et al. 23]

$$\begin{array}{lccc} \text{Probability densities} & \mathcal{P}(\mu) & \xrightarrow{P} & \mathcal{P}(\mu) \\ & \Gamma\big\downarrow & & \big\downarrow\Gamma \\ \text{Density operators} & \mathcal{Q}(H) & \xrightarrow{Q} & \mathcal{Q}(H) \end{array}$$

- Embedding of probability densities into quantum states on H:

$$\Gamma \colon \mathcal{P}(\mu) \to \mathcal{Q}(H), \quad \Gamma(\nu) = \rho := \langle \nu^{1/2}, \cdot \rangle \nu^{1/2}.$$

- Embedding of observables: $\pi \colon L^\infty(\mu) \to B(H)$, $(\pi f)g = fg$.
- Unitary evolution: $Q\rho = U^* \rho U$.
- Quantum–classical consistency:

$$\mathbb{E}_{P\nu} f = \mathbb{E}_{Q(\Gamma\nu)}(\pi f) \equiv \operatorname{tr}((Q(\Gamma\nu))(\pi f)).$$

Embedding dynamics into a quantum mechanical system

[G. 19; Freeman et al. 23]

Probability densities	$\mathcal{P}(\mu)$	$\xrightarrow{P}$	$\mathcal{P}(\mu)$
	$\Gamma \downarrow$		$\downarrow \Gamma$
Density operators	$\mathcal{Q}(H)$	$\xrightarrow{Q}$	$\mathcal{Q}(H)$
	$\mathbf{\Pi}'_L \downarrow$		$\downarrow \mathbf{\Pi}'_L$
Density matrices	$\mathcal{Q}(H_L)$	$\xrightarrow{Q_L}$	$\mathcal{Q}(H_L)$

- $H_L \subset H$: Finite-dimensional approximation space, $\Pi_L = \text{proj}_{H_L}$.
- Projection of quantum states:

$$\mathbf{\Pi}'_L(\rho) = \rho_L := \frac{\Pi_L \rho \Pi_L}{\text{tr}(\Pi_L \rho \Pi_L)}$$

- Projection of evolution operators:

$$Q_L \rho_L = U_L^{t*} \rho_L U_L, \quad U_L = \Pi_L U \Pi_L.$$

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Structure preservation

- Unlike a projection $\Pi_L \nu$ of a classical probability density, a projected quantum state $\Pi_L \rho \Pi_L$ is a positive operator.
- Embedding into the infinite-dimensional quantum system on H, and *then* projecting to finite dimensions, allows us to construct positivity-preserving approximation schemes in ways which are not possible in (commutative) function spaces.

Quantum mechanical closure

Original system	Parameterized system
$x_{n+1} = \Phi(x_n, \xi(y_n))$	$x_{n+1} = \tilde{\Phi}(x_n, \tilde{\xi}(\rho_n))$
$y_{n+1} = \Psi(x_n, y_n)$	$\rho_{n+1} = \tilde{\Psi}(x_n, \rho_n)$

- Resolved variables: $x_n \in \mathcal{X}$.
- Unresolved variables: $y_n \in \mathcal{Y}$.
- Full state space $X = \mathcal{X} \times \mathcal{Y}$.
- Fluxes from unresolved variables: $\xi \colon Y \to \mathbb{R}^d$, $\xi = (\xi_1, \dots, \xi_d)$.
- Surrogate unresolved variables (quantum states): $\rho_n \in \mathcal{Q}(H_L)$.
- Parameterized fluxes: $\tilde{\xi} \colon \mathcal{Q}(H_L) \to \mathbb{R}^d$, $\tilde{\xi} = (\tilde{\xi}_1, \dots, \tilde{\xi}_d)$,

$$\tilde{\xi}_k(\rho_n) = \operatorname{tr}(\rho_n(\pi \xi_k)).$$

- Evolution map for quantum states: $\tilde{\Psi} \colon \mathcal{X} \times \mathcal{Q}(H_L) \to \mathcal{Q}(H_L)$.

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Given: Samples $x_0, \dots, x_{N-1} \in \mathcal{X}$, $z_0, \dots, z_{N-1} \in \mathbb{R}^d$ with $z_n = \xi(y_n)$, along dynamical trajectory of the original system.

- Build data-driven basis $\{\phi_0, \dots, \phi_{L-1}\}$ of H_L.
- Compute $L \times L$ transfer operator matrix $\boldsymbol{P} = [P_{ij}]$,

$$P_{ij} = \langle \phi_i, P\phi_j \rangle.$$

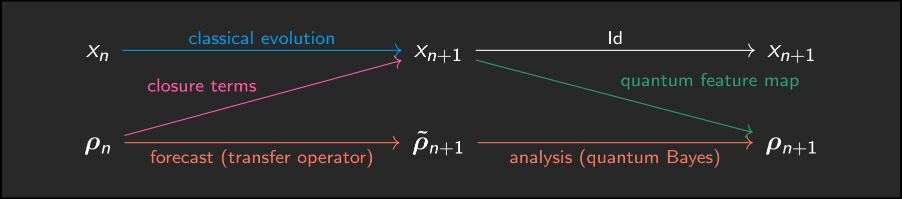
- Compute $L \times L$ multiplication operator matrices $\boldsymbol{\Xi}_1, \dots, \boldsymbol{\Xi}_d$,

$$\boldsymbol{\Xi}_k = [\Xi_{k,ij}], \quad \Xi_{k,ij} = \langle \phi_i, (\pi\xi_k)\phi_j \rangle.$$

- Construct matrix-valued feature map, $\boldsymbol{F} \colon X \to \mathbb{R}^{L \times L}$,

$$\boldsymbol{F}(x) = [F_{ij}(x)], \quad F_{ij}(x) = \langle \phi_i, \mathcal{F}_L(x)\phi_j \rangle.$$

Quantum mechanical closure



Closure algorithm

1. Compute parameterized fluxes: $\tilde{z}_n = (\tilde{z}_{n,1}, \ldots, \tilde{z}_{n,d})$, $z_{n,k} = \operatorname{tr}(\rho_n \Xi_k)$.
2. Update resolved variables: $x_{n+1} = \tilde{\phi}(x_n, z_n)$.
3. Compute prior quantum state: $\tilde{\rho}_{n+1} = \boldsymbol{P}\tilde{\rho}_n$.
4. Compute conditional state: $\rho_{n+1} = \tilde{\rho}_{n+1}|_{\boldsymbol{F}(x_{n+1})}$.

Lorenz 63

[after Palmer 01]

$$\dot{a}_1 = 2.3\,a_1 - 6.2\,a_3 - 0.49\,a_1 a_2 - 0.57\,a_2 a_3$$
$$\dot{a}_2 = -62 - 2.7\,a_2 + 0.49\,a_1^2 - 0.49\,a_3^2 + 0.14\,a_1 a_3$$
$$\dot{a}_3 = -0.63\,a_1 - 13\,a_3 + 0.43\,a_1 a_2 + 0.49\,a_2 a_3$$

- (a_1, a_2, a_3): PCA coordinates.
- Resolved variables: $(a_1, a_2) = x \in X \equiv \mathbb{R}^2$.
- Unresolved variables: $a_3 = y \in Y \equiv \mathbb{R}$.
- Flux terms: $\xi\colon Y \to \mathbb{R}$, $\xi(a_3) = a_3$.

Lorenz 63

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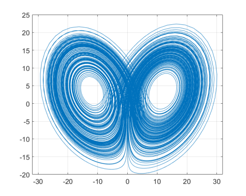
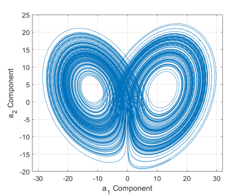
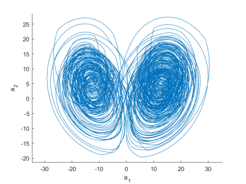
L63 system

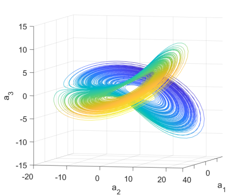
QM closure

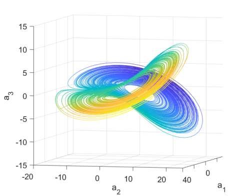
Gaussian closure

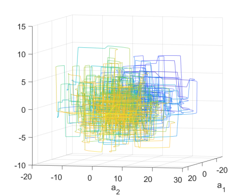












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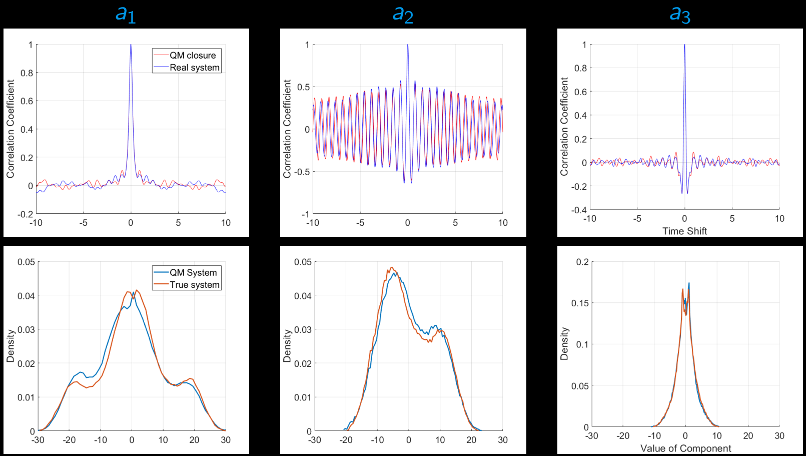

Quantum mechanical closure of PDE systems

Original system	Parameterized system
$x_{n+1} = \Phi(x_n, \xi(y_n))$	$x_{n+1} = \tilde{\Phi}(x_n, \tilde{\xi}(\rho_n))$
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- Spatial domain S equipped with measure ν.
- Full state space $X \equiv \mathcal{X} \times \mathcal{Y}$ is a function space, $X \subseteq L^2(S, \nu)$.
- Resolved state space $\mathcal{X}$ is a finite-dimensional subspace $\mathcal{X} \subset X$.
- Flux map $\xi \colon \mathcal{Y} \to L^2(S, \nu; \mathbb{R}^d)$.

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- Product state space $\Omega = X \times S$, $\sigma = \mu \times \nu$.
- Quantum mechanical Hilbert space

$$H_\Omega = L^2(\Omega, \sigma) \cong L^2(X, \mu) \otimes L^2(S, \nu) \cong L^2(X, \mu; L^2(S, \nu)).$$

- Field of quantum states: $\rho \in \tilde{\mathcal{Y}} \equiv L^2(S, \nu; \mathcal{Q}(H_\Omega))$.
- Fluxes represented by multiplication operators $\Xi_1, \ldots, \Xi_d : \in B(H_\Omega)$

$$\Xi_k f(x, y, s) = \xi_k(y)(s) \cdot f(x, y, s).$$

- Predicted flux components:

$$\tilde{\xi}_k(\rho)(s) = \operatorname{tr}(\rho(s)\Xi_k).$$

Factoring out dynamical symmetries

[G. et al. 19]

$$\begin{array}{ccc} \Omega & \xrightarrow{\Gamma_\Omega^g} & \Omega \\ {\scriptstyle F_\ell}\downarrow & \swarrow {\scriptstyle F_\ell} & \\ \mathbb{R}^\ell & & \end{array}$$

- Spatial domain S with action $\Gamma_S^g \colon S \to S$, $g \in G$, of a symmetry group G.
- There is a (right) action $\Gamma_X^g \colon X \to X$ on $X \subset L^2(S, \nu)$,

$$\Gamma_X^g(x) = x \circ \Gamma_Y^{-g}.$$

- Γ_X^g is a dynamical symmetry if:

$$\Gamma_X^g \circ T = T \circ \Gamma_X^g, \quad \forall g \in G.$$

Factoring out dynamical symmetries

[G. et al. 19]

$$
\begin{array}{ccc}
\Omega & \xrightarrow{\Gamma^g_\Omega} & \Omega \\
{\scriptstyle F_\ell}\downarrow & \swarrow {\scriptstyle F_\ell} & \\
\mathbb{R}^\ell & &
\end{array}
$$

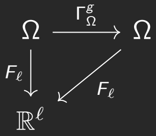
- Define delay-coordinate map $F_\ell \colon \Omega \to \mathbb{R}^{m\ell}$, $m = \dim \mathcal{X}$, as

$$F_\ell(x, y, s) = \left(x(s), T(x)(s), \dots, T^{\ell-1}(x)(s)\right).$$

- Then $f \circ F_\ell \in H_\Omega$ is invariant under the symmetry group action $\Gamma^g_\Omega = \Gamma^g_X \times \Gamma^g_Y$.

Factoring out dynamical symmetries

[G. et al. 19]



- Fix a kernel $k_\ell \colon \mathbb{R}^{m\ell} \times \mathbb{R}^{m\ell} \to \mathbb{R}$ with corresponding integral operator $K_\ell \colon H_\Omega \to H_\Omega$,

$$K_\ell f = \int_\Omega k_\ell(F_\ell(\cdot), F_\ell(x, y, s)) f(x, y, s) \, d\sigma(x, y, s).$$

- Compute eigendecomposition of K_ℓ to obtain equivariant basis functions $\phi_j \in L^2(\Omega, \sigma)$,

$$K_\ell \phi_j = \lambda_j \phi_j, \quad \mathcal{U}^g \circ \phi_j = \phi_j \circ \Gamma_X^g,$$

where $\mathcal{U}^g \colon L^2(S, \nu) \to L^2(S, \nu)$ is the composition operator

$$T_S^g f = f \circ \Gamma_S^g.$$

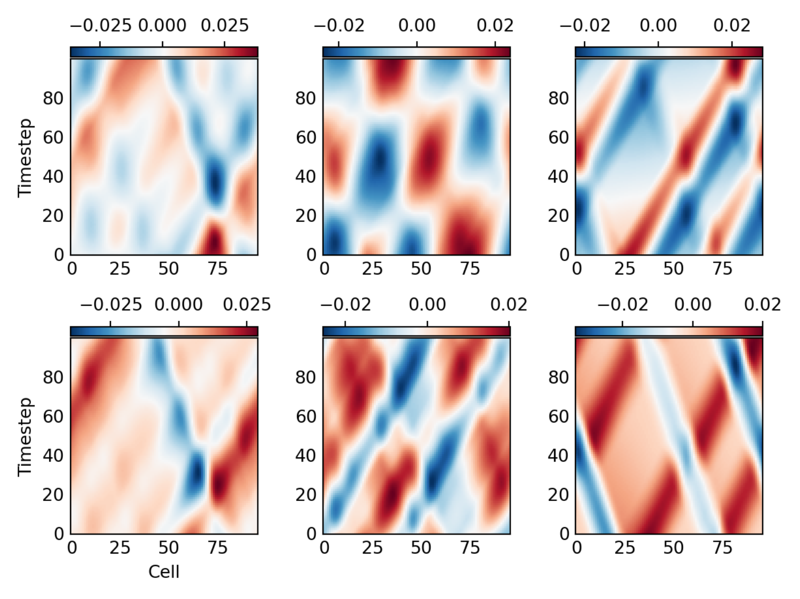
QM closure of the shallow-water equations

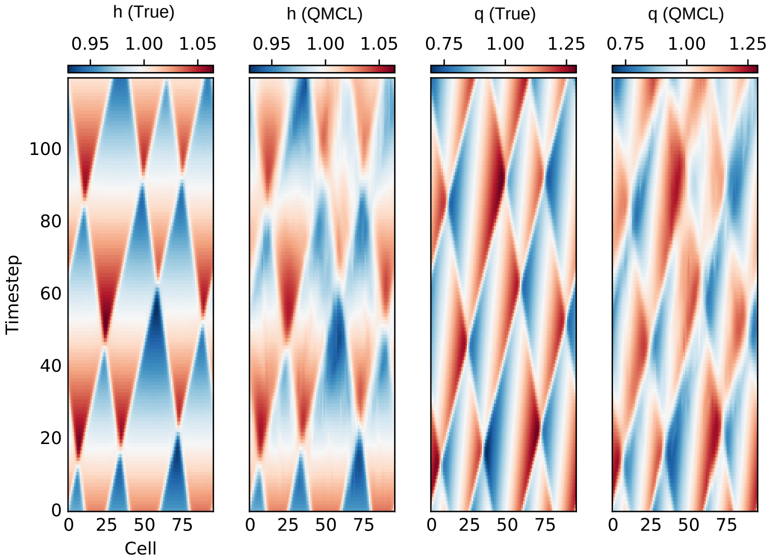
[Vales et al. 25; after Timofeyev et al. 24]

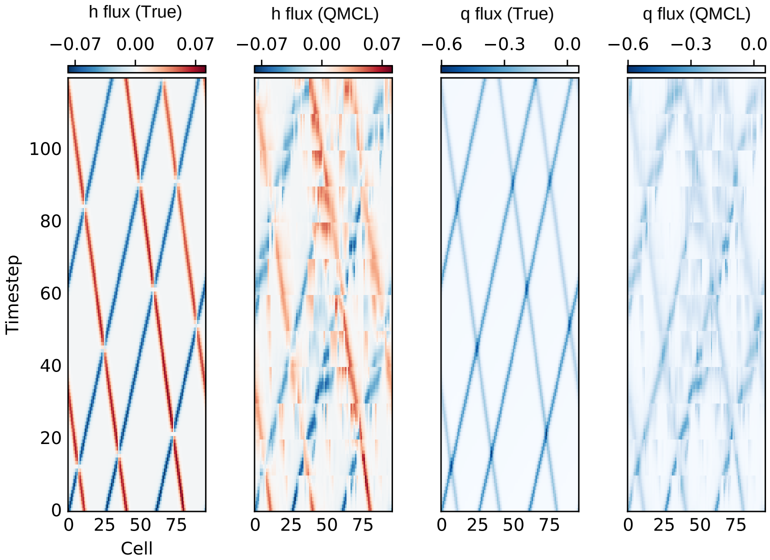
$$\partial_t h + \partial_x q = 0, \quad \partial_t q + \partial_x \left(\frac{q^2}{h} + \frac{h^2}{2\,\mathrm{Fr}^2} \right) = 0$$

- Fine mesh finite volume discretization: $\hat{x}_j$.
- Local spatial averaging (resolved variables): $x_j = \frac{1}{K} \sum_k \hat{x}_k$.
- 1920 fine cells, 96 coarse cells, 300 time samples on 3 trajectories.
- Basis size $L = 6144$.

Basis functions ϕ_j




h (True)
h (QMCL)
q (True)
q (QMCL)
0.95
1.00
1.05
0.75
1.25
Timestep
0
20
40
60
80
100
25
50
75
Cell



h flux (True)
h flux (QMCL)
q flux (True)
q flux (QMCL)
−0.07 0.00 0.07
−0.07 0.00 0.07
−0.6 −0.3 0.0
−0.6 −0.3 0.0
Timestep
0 20 40 60 80 100
Cell
0 25 50 75

Summary and outlook

- Koopman/transfer operator techniques combined with quantum theory lead to closure schemes with useful structure-preservation properties.
  - Positivity of observables.
  - Dynamical symmetries
- Methods are amenable to data-driven approximation with convergence guarantees.

Future directions

- Use kernel learning to optimize quantum Bayesian update.
- Explore quantum circuit implementations.

References

[1] D. C. Freeman, D. Giannakis, B. Mintz, A. Ourmazd, and J. Slawinska, "Data assimilation in operator algebras," *Proc. Natl. Acad. Sci.*, vol. 120, no. 8, e2211115120, 2023. DOI: 10.1073/pnas.2211115120.

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