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Quantum Mechanics for Large-Eddy Parameterizations

Quantum mechanical closure (QMCl) of a cloud-resolving EULAG atmosphere model

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We also thank our collaborator Andrzej Wyszogrodski

I · QUANTUM MECHANICS AS PROBABILITY

Non-commutative analogs of objects in classical probability theory

STATES $\rho \in B(H) : \rho \geq 0,\ \mathrm{tr}\,\rho = 1$

Analogous conditions to classical probability distribution

OBSERVABLES $A = A^* \in B(H)$

Spectra determine observable range

EXPECTATION $\langle A \rangle_\rho = \mathrm{tr}(A\rho)$

Used for observable measurement

BAYES UPDATE $\rho \,|\, E \;\mapsto\; \dfrac{E\rho E}{\mathrm{tr}(E\rho E)}$

Quantum analog to Bayes' rule

- Densities embed as diagonal states; off-diagonals encode "quantum behavior"

General dynamical closure: a surrogate system & flux map

FULL SYSTEM $\Phi : \Omega \to \Omega, \quad \Omega = \mathcal{X} \times \mathcal{Y}$

State space broke into resolved and unresolved components

FLUX MAP $P_{\mathcal{X}} \circ \Phi(\omega) = \varphi(x, Z(y)), \quad \omega = (x, y)$

Flux map determines effect of unresolved components on resolved dynamics

SURROGATE $\tilde{\Phi}(x, \tilde{y}) = \big(\varphi(x, \tilde{Z}(\tilde{y})),\ \tilde{\psi}(x, \tilde{y})\big), \quad \tilde{\Omega} = \mathcal{X} \times \tilde{\mathcal{Y}}$

Establish surrogate unresolved state space, dynamics, and flux map

II · KOOPMAN & THE QMCL EMBEDDING

KOOPMAN $U^t f = f \circ \Phi^t \quad \text{on } L^2(\mu)$

Dual of transfer operator

PROJECTION $\mathbf{\Pi}_L(A) = \Pi_L\, A\, \Pi_L$

Compression of an operator to the finite subspace

ASSOC. MAP $\pi : L^\infty(\mu) \to B(L^2(\mu)), \quad (\pi f)\, g = f g$

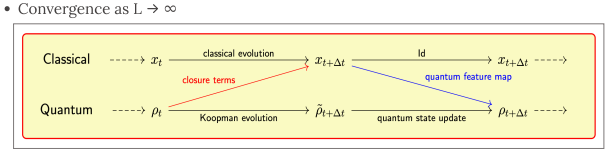
Observable association: functions become multiplication operators

KOOPMAN CONJ. $\mathcal{U}^t A = U^t\, A\, (U^t)^*$

Evolution of quantum observables by Koopman conjugation

$$\begin{tikzcd} L^\infty(\mu) \arrow[r, "U^t"] \arrow[d, "\pi"] & L^\infty(\mu) \arrow[d, "\pi"] \\ B(L^2(\mu)) \arrow[r, "\mathcal{U}^t"] & B(L^2(\mu)) \end{tikzcd}$$

- **Positivity preservation** for observables
- Can be mapped to **quantum circuitry**
- Convergence as L → ∞



III · NUMERICAL IMPLEMENTATION

- QMCl objects generated from **time-ordered training set**, converging for measure-preserving, compactly-supported ergodic systems as N, L grow

TRAINING DATA $\omega_0, \omega_1, \ldots, \omega_{N-1}, \quad \omega_{n+1} = \Phi^{\Delta t}(\omega_n)$

Time ordered fully-resolved snapshots

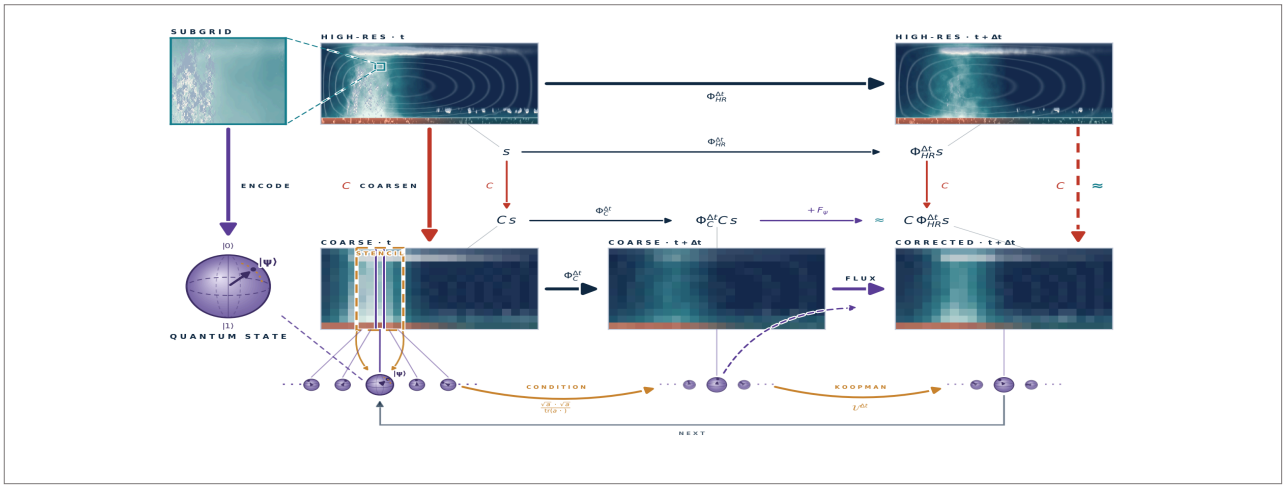
BASIS OF L² $K\varphi_l = \lambda_l \varphi_l, \quad H_L = \mathrm{span}\{\varphi_0, \ldots, \varphi_{L-1}\}$

Kernel integral operator extracts geometric structure

OPERATORS $[U]_{ij} = \langle \varphi_i, U^{\Delta t} \varphi_j \rangle, \quad [A]_{ij} = \langle \varphi_i, a\, \varphi_j \rangle$

Projection onto learned eigenbasis

IV · THE CLOSURE STRUCTURE



DYNAMICS $\omega_{HR}^{t+dt} = \Phi^{dt}(\omega_{HR}^t), \qquad \omega_C^{t+dt} = \Phi_C^{dt}(\omega_C^t)$

AVERAGED FLUX $r^\psi = \frac{1}{dt}\left[\, g^\psi(C \circ \Phi^{dt}\omega) - g^\psi(\Phi_C^{dt}\, C\omega)\,\right]$

Error term between high-res and coarse model evolution

COUPLED STEP $\Phi_{QM}^{dt}(\bar{\omega}, \rho) = \Phi_C^{dt}(\bar{\omega}) + dt \cdot R_\omega \approx C \circ \Phi^{dt}(\omega)$

Inject flux to fix averaged dynamics

EULAG-QMCL CIRCUIT $\bar{\psi}^{n+1} = \mathrm{MPDATA}\big(\bar{\psi}^n + \frac{\Delta t}{2} F^n,\ \bar{v}\big) + \frac{\Delta t}{2} F^{n+1} + \Delta t\, f^\psi$

EULAG advection process - Prusa, Smolarkiewicz & Wyszogrodzki, Comput. Fluids *37 (2008);*
Colored term is the injected QMCl flux

The flux term carries subgrid-scale dynamical contributions

V · SET-UP: FLUXES AS OBSERVABLES

- Quantum observables trained on residual terms
- One pure state per model column, conditioned on a 9-column horizontal stencil

FLUX MAP $A_{(x,z)}^\psi = \pi\big(r_{(x,z)}^\psi\big)$

Quantum observable is the association map applied to the residual

COLUMN STATES $\rho_x, \quad x = 1, \ldots, N_x$

Separate quantum state for each vetical column

STENCIL $\rho_x \,|\, \bar{\omega}_{x-4}, \ldots, \bar{\omega}_{x+4}$

Conditioning on a 9-column horizontal stencil

VI · WALKER-CELL IMPLEMENTATION

- 2-D anelastic EULAG in the x–z plane; periodic horizontal boundaries
- 1000 km domain — fine: dx = 1 km (n_x = 1000); coarse: dX = 10 km (N_x = 100); n_z = 51
- Quasi-periodic deep convection; chaotic turbulence in the convective center
- Training: 10,000 steps ≈ 1 day; L = 500

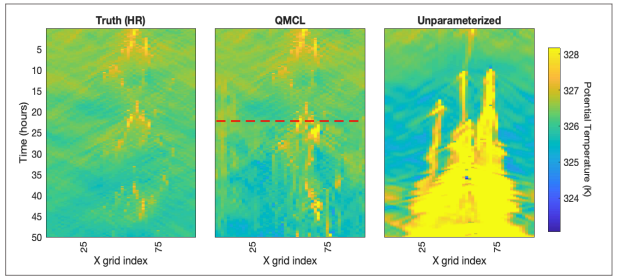


Fig. 1. Unparameterized coarsening: convection collapses. QMCl model retains convective structure. Red line indicates end of in-sample time regime.

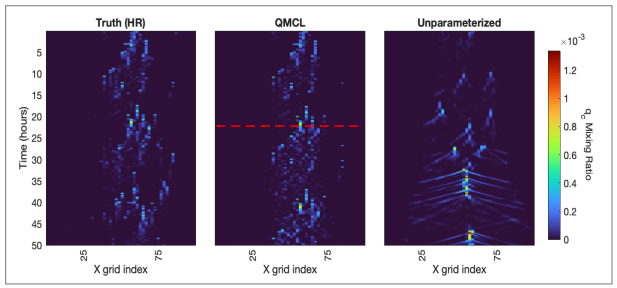


Fig. 2. QMCl reproduces cloud distribution and periodicity.