Data Assimilation for multiscale models

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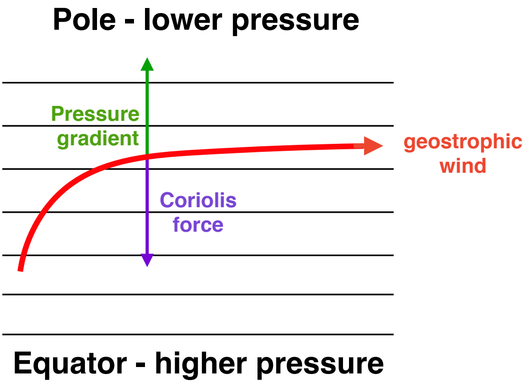
Motivation

Multiscale models often preserve balances, e.g. geostrophic balance in atmospheric models



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Multiscale Hamiltonian model

Hamiltonians:

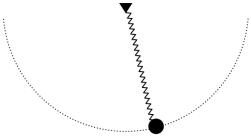
$$H^{\varepsilon}(q,p) = \frac{1}{2}p^{\mathrm{T}}p + \frac{1}{2\varepsilon^2}g(q)^{\mathrm{T}}Kg(q) + V(q)$$
$$H^{\varepsilon}_{\mathrm{osc}}(q,p) = \frac{1}{2}(G(q)p)^{\mathrm{T}}(G(q)G(q)^{\mathrm{T}})^{-1}G(q)p + \frac{1}{2\varepsilon^2}g(q)^{\mathrm{T}}Kg(q)$$

Equations of motion:

$$\dot{q} = p$$
$$\dot{p} = -\varepsilon^{-2}G(q)^{\mathrm{T}}Kg(q) - \nabla_q V(q),$$

Slow manifold:

$$g(q) \approx 0$$



Problem

Transformation of forecast ensemble into analysis ensemble

$$z_{\mathrm{a}}^{j}(t) = \sum_{i=1}^{M} z_{\mathrm{f}}^{i}(t) d_{ij}(t) \qquad \text{(LETF)}$$

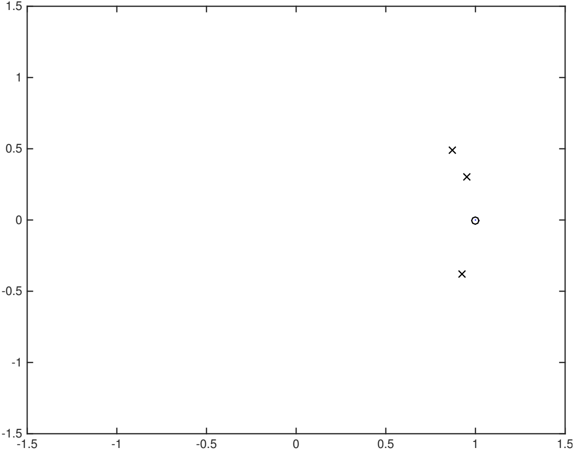
apply the same transformation to the forecast values of g

$$g_{\mathrm{a}}^{j}(t) = \sum_{i=1}^{M} g_{\mathrm{f}}^{i}(t) d_{ij}(t)$$

note:

$$g_{\mathrm{a}}^{j}(t) \neq g(z_{\mathrm{a}}^{j}(t)) \quad \text{in general}$$

Example: Stiff Spring Pendulum



Strategy 1 - Kalman-Bucy with pseudo observations (1)

solve a minimisation problem:

$$(z^j)^* = \underset{z}{\operatorname{argmin}} \left\{ (z - z_{\mathrm{a}}^j)^{\mathrm{T}} (P_{zz}^{\mathrm{a}})^{-1} (z - z_{\mathrm{a}}^j) + \right.$$
$$\left. (g(z) - \gamma g_{\mathrm{a}}^j)^{\mathrm{T}} R^{-1} (g(z) - \gamma g_{\mathrm{a}}^j) \right\}$$

Strategy 1 - Kalman-Bucy with pseudo observations (2)

solve minimisation via pseudo dynamics:

$$\frac{\mathrm{d}}{\mathrm{d}s} z^j = -P_{zg} R^{-1} \left(g(z^j) - \gamma g_{\mathrm{a}}^j \right), \qquad j = 1, \ldots, M$$

$$\text{with} \quad P_{zg} = \frac{1}{M-1} \sum_i z^i (g(z^i) - \bar{g})^{\mathrm{T}}$$

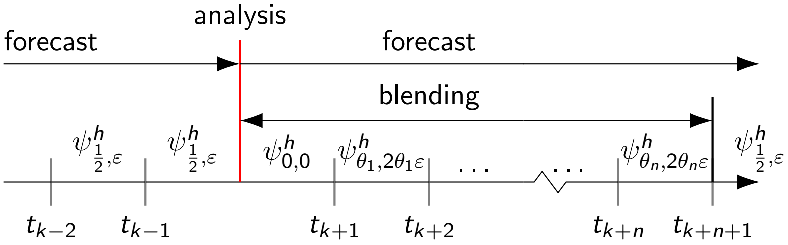
- R could be $P_{gg} = \frac{1}{M-1} \sum_{i=1}^{M} g(z_i)(g(z_i) - \bar{g})^T$
- $0 \leq \gamma \leq 1$
- stop when $\|g(z^j) - \gamma g_{\mathrm{a}}^j\| \leq \mathrm{tol}$

Strategy 2 - Blending

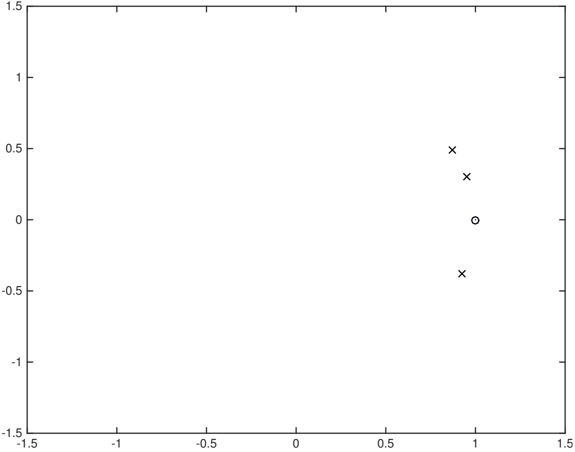
Blending numerical scheme

$$z^{n+1} = \psi^h_{\theta,\varepsilon}(z^n, z^{n+1}) \quad \theta \in [0, 1/2] \quad \text{which}$$

- enforces discrete balance $0 = g(\psi^h_{0,0}(z^n))$ for $\theta = 0$ and
- preserves the energy $H(z^n) = H(\psi^h_{\frac{1}{2},\varepsilon}(z^n))$ for $\theta = \frac{1}{2}$.



Example: Pendulum with balancing



A - Stiff spring double pendulum

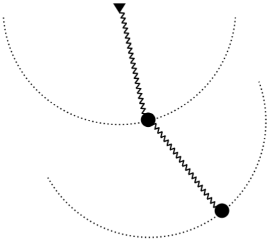
$$H^{\varepsilon}(q,p) = \frac{1}{2}p^{\mathrm{T}}p + \frac{1}{2\varepsilon^2}g(q)^{\mathrm{T}}\begin{pmatrix}1 & 0\\ 0 & 0.04\end{pmatrix}g(q) + \begin{pmatrix}0\\10\\0\\10\end{pmatrix}^{\mathrm{T}} q$$

Bounded first derivatives: $\dot{q}^{\varepsilon}, \dot{p}^{\varepsilon} = \mathcal{O}(\varepsilon^0)$

$\Rightarrow g(q^{\varepsilon}(t)) = \mathcal{O}(\varepsilon^2)$

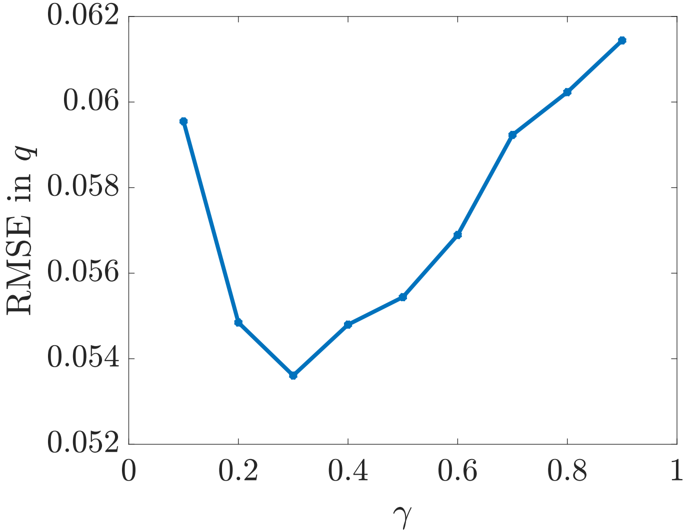
$\Rightarrow H^{\varepsilon}_{\mathrm{osc}}((q^{\varepsilon}(t), p^{\varepsilon}(t)) = \mathcal{O}(\varepsilon^2)$

$\Rightarrow G(q^{\varepsilon}(t))p^{\varepsilon}(t) = O(\varepsilon)$

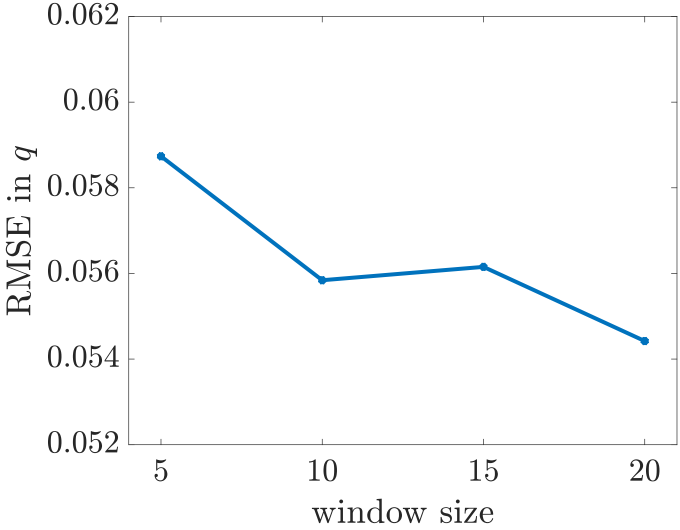


Toy model for balanced flow regimes
in atmosphere-ocean dynamics

Numerical result Kalman-Bucy



Numerical result Blending



B - Thermally embedded spring pendulum

$$H^\varepsilon(q,p) = \frac{1}{2}p^{\mathrm{T}}p + \frac{1}{2\varepsilon^2}g(q)^2, \quad g(q) = \sqrt{q^{\mathrm{T}}\begin{pmatrix}1 & 0\\ 0 & \alpha^2\end{pmatrix}q} - 1$$

Equations of motion:

$$\begin{aligned}\dot{q} &= p\\ \dot{p} &= -\varepsilon^{-2}G(q)^{\mathrm{T}}g(q) - \beta p + \sqrt{2\beta k_B T}\dot{W}\end{aligned}$$

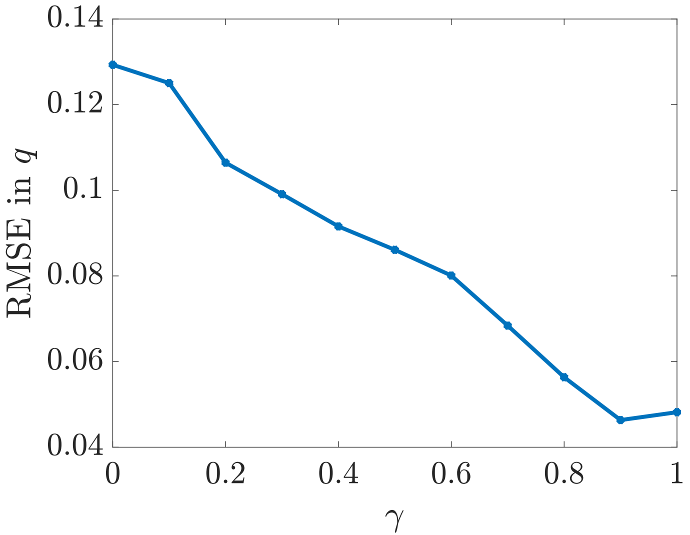
$\mathbb{E}[H^\varepsilon(q,p)] = \mathcal{O}(\varepsilon^0)$

action variable: $J^\varepsilon(q,p) = \frac{H^\varepsilon_{\mathrm{osc}}(q,p)}{\omega^\varepsilon(q)}, \quad \omega^\varepsilon(q) = \varepsilon^{-1}\sqrt{G(q)G(q)^{\mathrm{T}}}$

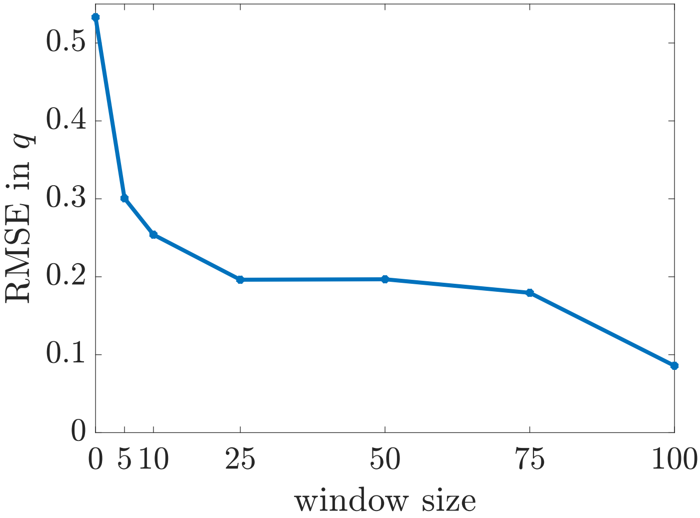
correction term: $F_{\mathrm{corr}}(q) = -J^\varepsilon(q,p)\nabla_q\omega^\varepsilon(q)$

Langevin dynamics for molecular dynamics simulations

Numerical result Kalman-Bucy



Numerical result Blending



(regularised) Shallow water equations (1)

Model:

$$\frac{Du}{Dt} = f^0 v - g^0 \tilde{H}_x$$
$$\frac{Dv}{Dt} = -f^0 u - g^0 \tilde{H}_y$$
$$\frac{\partial H}{\partial t} = -\nabla \cdot \begin{pmatrix} Hu \\ Hv \end{pmatrix}$$

with

$$\tilde{H} = \left[1 - \alpha^2 \Delta\right]^{-1} \left(H - \frac{\alpha^2}{g^0}(f^0 \zeta - 2J) \right)$$
$$\zeta = v_x - u_y, \quad J = v_x u_y - u_x v_y$$

additional cause of imbalance: Localisation

(regularised) Shallow water equations (2)

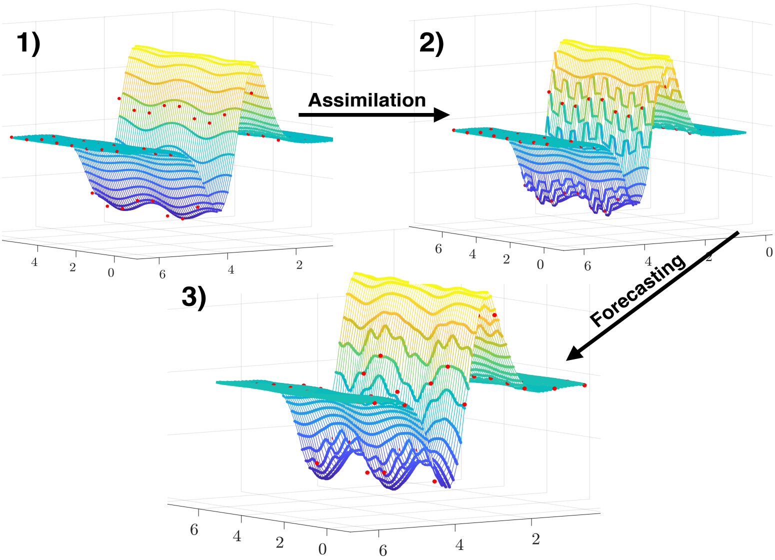
Balance equations:

$$\delta_1 = g^0(H - \tilde{H}) = \alpha^2 \left[1 - \alpha^2 \Delta\right]^{-1} \left(g^0 \Delta H - f^0 \zeta + 2J\right)$$
$$\delta_2 = \nabla \cdot \begin{pmatrix} u \\ v \end{pmatrix} = u_x + v_y,$$

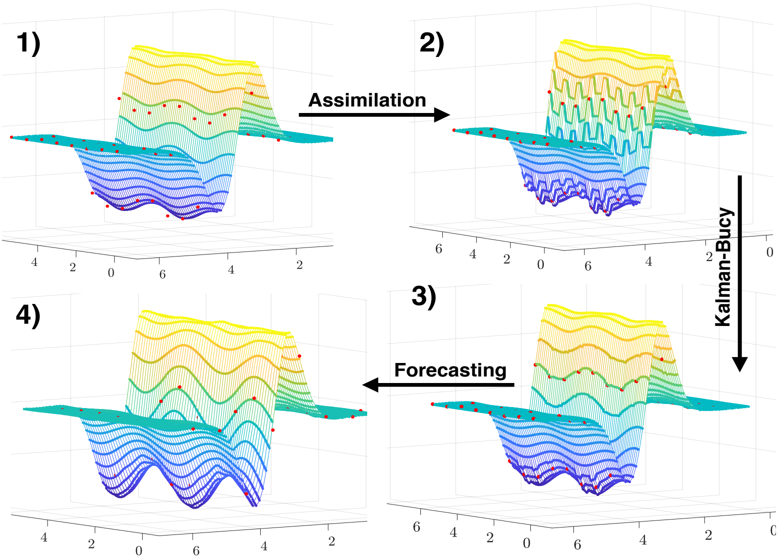
Choice of R for Kalman-Bucy:

$$R := \begin{pmatrix} 1 - \alpha^2 \Delta & 0 \\ 0 & \mathrm{diag}(P_{\delta_2 \delta_2}) \end{pmatrix}$$

Numerical result - without Kalman-Bucy



Numerical result - with Kalman-Bucy



Conclusion

- Multiscale models preserve balance relations
- Data assimilation step is a linear transformation
- Nonlinear balance is destroyed by data assimilation
- leading to fast oscillations and unphysical predictions
- Two stragegies to deal with that
  - Kalman-Bucy pseudo dynamics applied after assimilation step
  - Blending between limit and full model in the forecasting step
- *Balanced data assimilation for highly-oscillatory mechanical systems, M. Reinhardt, G. Hastermann, R. Klein, S. Reich, 2017, arXiv:1708.03570*

Thank you!!