# Early Steps in Data Assimilation

Ocean Current Modeling

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# Governing Equations

form my perspective

We want to solve these equations

$$\frac{\partial q_k}{\partial t} + J(\psi_k, q_k) = -\frac{1}{\tau_d}(-1)^k(\psi_1 - \psi_2 - \psi_R) - \frac{1}{\tau_f}\delta_{k2}\nabla^2\psi_k - \nu\nabla^8 q_k$$
$$q_i = \nabla^2\psi_i + (-1)^k(\psi_1 - \psi_2) + \beta y \tag{1}$$

For a system which has two layers ($k = 1, 2$).

## What is this equation?

- called Potential Vorticity (PV) equation,
- $q$ is PV,
- $\psi$ is geostrophic stream function,
- $k$ represent each layer.
- Let's make it understandable for Engineers and Mathematicians.

# Governing Equations

form my perspective

- $Z_0$ is the water surface, $h_B$ is the bottom of the ocean and $Z_1$ is the interface between the two layers,
- in each layer, density is constant,
- in each layer, pressure varies hydrostatically,

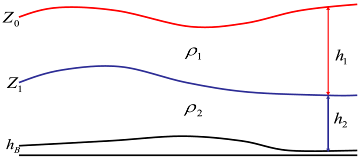


Figure: chematic of the two-layer shallow water system

# Governing Equations

form my perspective

- in each layer, pressure varies hydrostatically,

$$\begin{aligned} p_1 &= \rho_1 g(Z_0 - z) \\ p_2 &= \rho_1 g(Z_0 - Z_1) + \rho_2 g(Z_1 - z) \end{aligned} \tag{2}$$

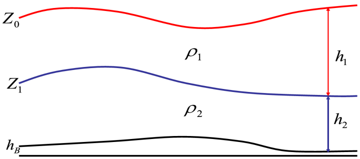


Figure: chematic of the two-layer shallow water system

# Governing Equations

form my perspective

- in each layer, pressure varies hydrostatically,

$$\begin{aligned} p_1 &= \rho_1 g (Z_0 - z) \\ p_2 &= \rho_1 g (Z_0 - Z_1) + \rho_2 g (Z_1 - z) \end{aligned} \tag{3}$$

The momentum equation becomes:

$$\begin{aligned} \frac{D\vec{u}_1}{Dt} + f \times \vec{u}_1 &= -\frac{1}{\rho_1} \nabla p_1 = -g \nabla Z_0 \\ \frac{D\vec{u}_2}{Dt} + f \times \vec{u}_2 &= -\frac{1}{\rho_2} (\rho_1 g \nabla Z_0 - \rho_2 g \nabla Z_1) \end{aligned} \tag{4}$$

Here, $f$ is Coriolis acceleration.

# Governing Equations

form my perspective

## Momentum equation

$$\frac{D\vec{u}_1}{Dt} + f \times \vec{u}_1 = -\frac{1}{\rho_1}\nabla p_1 = -g\nabla Z_0$$
$$\frac{D\vec{u}_2}{Dt} + f \times \vec{u}_2 = -\frac{1}{\rho_2}(\rho_1 g\nabla Z_0 - \rho_2 g\nabla Z_1) \tag{5}$$

Taking curl of momentum equation:

$$\frac{\partial \xi_i}{\partial t} + \vec{u}_i.\nabla(\xi_i + f) = -(\xi_i + f)\nabla.\vec{u}_i \tag{6}$$

The vorticity equation will be same for both layers.

# Governing Equations

form my perspective

The conservation of mass equation:

$$\begin{aligned}
&\frac{D}{Dt}(M_i) = 0 \\
&\frac{D}{Dt}(M_i) = \frac{D}{Dt}(\rho_i h_i A) = \rho_i \frac{D}{Dt}(h_i A) = 0 \\
&A\frac{Dh_i}{Dt} + h_i \frac{DA}{Dt} = 0
\end{aligned} \tag{7}$$

using material derivative $\frac{DA}{Dt} = A\nabla.\vec{u}_i$, we will have:

$$\frac{Dh_i}{Dt} + h_i \nabla.\vec{u}_i = 0 \tag{8}$$

# Governing Equations

form my perspective

**We have**

$$\frac{\partial \xi_i}{\partial t} + \vec{u}_i . \nabla (\xi_i + f) = -(\xi_i + f) \nabla . \vec{u}_i \tag{9}$$

$$\frac{Dh_i}{Dt} + h_i \nabla . \vec{u}_i = 0 \tag{10}$$

Combining these two equations:

$$\frac{D(\xi_i + f)}{Dt} = \frac{\partial \xi_i}{\partial t} + \vec{u}_i . \nabla (\xi_i + f) = \frac{\xi_i + f}{h_i} \frac{Dh_i}{Dt} \tag{11}$$

Or

$$\frac{Dq_i}{Dt} = \frac{D}{Dt} \left( \frac{\xi_i + f}{h_i} \right) = 0 \tag{12}$$

This is potential vorticity conservation for the two layer case.

# Governing Equations

form my perspective

The next step is to apply Quasi-Geostrophic scaling to this equation. For this purpose we need to consider following assumptions:

- The Rossby number is small, $\vec{u}_a/\vec{u}_g \sim O(R_o)$,
- We can write $h_i = H_i + h_i'$, where $h_i'/H_i \sim O(R_o)$,
- $f = f_0 + \beta y$, where $\beta y/f_0 \sim R_o$,
- Advection is dominatied by geostrophic velocity, $D/Dt = \partial/\partial_t + u_g\partial/\partial_x + v_g\partial/\partial_y$.

**What is Geostrophic?**

$$\frac{D\vec{u}_1}{Dt} + f \times \vec{u}_1 = -g\nabla Z_0$$
$$f \times \vec{u}_{1,g} = -g\nabla Z_0 \tag{13}$$

## Governing Equations

form my perspective

$$\frac{D}{Dt}\left(\frac{\xi_i + f}{h_i}\right) = 0 \tag{14}$$

We use Taylor expansion

$$\begin{aligned}\frac{\xi_i + f}{H_i + h_i'} &= \frac{\xi_i + f}{H_i}\left(1 + \frac{h_i'}{Hi}\right)^{-1} \\ &= \frac{1}{H_i}\left(\xi_i + f - \frac{\xi_i h_i'}{H_i} - f\frac{h_i'}{H_i}\right) \\ &= \frac{1}{H_i}\left(\xi_i + f_0 + \beta y - \frac{\xi_i h_i'}{H_i} - (f_0 + \beta y)\frac{h_i'}{H_i}\right)\end{aligned} \tag{15}$$

Using the assumptions and this equation, one can gather first order terms as

$$\frac{Dq_i}{D_t} = 0; \qquad q_i = \xi_{gi} + \beta y - f_0\frac{h_i'}{H_i} \tag{16}$$

## Governing Equations

form my perspective

Zero Order will result in Geostrophic balance.

First Order

$$\frac{Dq_i}{D_t} = 0; \qquad q_i = \xi_{gi} + \beta y - f_0 \frac{h_i'}{H_i} \tag{17}$$

From Geostrophi balance we have

$$\begin{aligned}
& f_o \times \vec{u}_1 = -g \nabla Z_0 \\
& f_o \times \vec{u}_2 = -g \nabla Z_0 - g' \nabla Z_1 \\
& Z_0 = h_1 + h_2 + h_B; \quad Z_1 = h_2 + h_B; \qquad u_x = -\partial_y \psi; \quad u_v = \partial_x \psi \\
& \psi_1 = \frac{g}{f_o}(h_1' + h_2' + h_B) \\
& \psi_2 = \frac{g}{f_o}(h_1' + h_2' + h_B) + \frac{g'}{f_o}(h_2' + h_B)
\end{aligned} \tag{18}$$

# Governing Equations

form my perspective

$$
\begin{aligned}
q_i &= \xi_{gi} + \beta y - f_0 \frac{h_i'}{H_i} \\
\psi_1 &= \frac{g}{f_o}(h_1' + h_2' + h_B) \\
\psi_2 &= \frac{g}{f_o}(h_1' + h_2' + h_B) + \frac{g'}{f_o}(h_2' + h_B)
\end{aligned} \tag{19}
$$

$$
\begin{aligned}
h_1' &= \frac{f_o}{g}\psi_1 + \frac{f_o}{g'}(\psi_1 - \psi_2) \\
h_2' &= \frac{f_o}{g'}(\psi_2 - \psi_1) - h_B
\end{aligned} \tag{20}
$$

# Governing Equations

form my perspective

$$g' = \frac{\rho_2 - \rho_1}{\rho_1}; \qquad \frac{g'}{g} \ll 1$$
$$\xi_i = \nabla^2 \psi_i \tag{21}$$

$$\frac{Dq_1}{Dt} = 0; \qquad q_1 = \nabla^2\psi_1 + \beta y - \frac{f_0^2}{H_1 g'}(\psi_1 - \psi_2)$$
$$\frac{Dq_2}{Dt} = 0; \qquad q_2 = \nabla^2\psi_2 + \beta y - \frac{f_0^2}{H_2 g'}(\psi_2 - \psi_1) - \frac{f_o h_B}{H_2} \tag{22}$$
$$\frac{Dq_i}{Dt} = \frac{\partial q_i}{\partial t} + \vec{u}_g . \nabla q_i = \partial_t q_i - \partial_y \psi_i \, \partial_x q_i + \partial_x \psi_i \, \partial_y q_i = 0$$
$$\partial_t q_i + J(\psi_i, q_i) = 0$$

# Governing Equations

form my perspective

## Where we started?

$$\partial_t q_k + J(\psi_k, q_k) = -\frac{1}{\tau_d}(-1)^k(\psi_1 - \psi_2 - \psi_R) - \frac{1}{\tau_f}\delta_{k2}\nabla^2\psi_k - \nu\nabla^8 q_k$$
$$q_i = \nabla^2\psi_i + (-1)^k(\psi_1 - \psi_2) + \beta y \tag{23}$$

## Where are we?

$$\partial_t q_k + J(\psi_k, q_k) = 0$$
$$q_1 = \nabla^2\psi_1 + \beta y - \frac{f_0^2}{H_1 g'}(\psi_1 - \psi_2) \tag{24}$$
$$q_2 = \nabla^2\psi_2 + \beta y - \frac{f_0^2}{H_2 g'}(\psi_2 - \psi_1) - \frac{f_o h_B}{H_2}$$

# Governing Equations

form my perspective

$$q_i = \nabla^2\psi_i + \beta^* y + (-1)^k(\psi_1 - \psi_2)$$
$$q_1 = \nabla^2\psi_1 + \beta y - \frac{f_0^2}{H_1 g'}(\psi_1 - \psi_2)$$

The main equation is dimensionless. We use:

- $\lambda = \sqrt{gD}/f$ (Rossby radius of deformation) for the length scale,
- $\lambda/U$ for the time scale,

For specific case we will study here, we assume $U = 40\, ms^{-1}$ and $D = 500\, m$. Therefore,

$$\hat{L} = \lambda = 700\, km \qquad \hat{T} \sim 4.86\, h \tag{25}$$

## Governing Equations

form my perspective

$$q_i = \nabla^2\psi_i + \beta^* y + (-1)^k(\psi_1 - \psi_2)$$
$$q_1 = \nabla^2\psi_1 + \beta y - \frac{f_0^2}{H_1 g'}(\psi_1 - \psi_2)$$

$$f = 2\Omega\, sin\phi; \qquad \Omega = 7.292115 \times 10^{-5} s^{-1}$$
$$f = f_0 + \beta y = (2\Omega\, sin\phi_0) + (2\Omega\, cos\phi_0)\, y \tag{26}$$

at $\phi = 45^o$

$$f_0 = 1 \times 10^{-4} s^{-1} \qquad \beta = 1.6 \times 10^{-11} m^{-1} s^{-1}$$
$$\beta^* = \frac{\beta\lambda^2}{U} = 0.196 \tag{27}$$

# Governing Equations

form my perspective

## Where we started?

$$\partial_t q_k + J(\psi_k, q_k) = -\frac{1}{\tau_d}(-1)^k(\psi_1 - \psi_2 - \psi_R) - \frac{1}{\tau_f}\delta_{k2}\nabla^2\psi_k - \nu\nabla^8 q_k$$
$$q_i = \nabla^2\psi_i + (-1)^k(\psi_1 - \psi_2) + \beta y \tag{28}$$

What are the other terms?

- Radiative processes in an idealized fashion as Newtonian relaxation of temperatures to ward an axially and hemispherically symmetric radiative equilibrium state,
- linear bottom friction,
- Biharmonic diffusion is also used to prevent the enstrophy pileup at smaller scales (stability).

# Toy problem

settings

## Where we started?

$$\partial_t q_k + J(\psi_k, q_k) = -\frac{1}{\tau_d}(-1)^k(\psi_1 - \psi_2 - \psi_R) - \frac{1}{\tau_f}\delta_{k2}\nabla^2\psi_k - \nu\nabla^8 q_k \quad (29)$$

We had

$$\hat{L} = \lambda = 700\,km \qquad \hat{T} \sim 4.86\,h \qquad \beta^* = \frac{\beta\lambda^2}{U} = 0.196$$

For the rest of variables

$$\tau_d = 100 \qquad \tau_f = 15 \qquad \nu = 0.01 \quad (30)$$

$$-\frac{\partial\psi_R}{\partial y} = sech\left(\frac{y}{\sigma}\right) \qquad \sigma = 3.5 \quad (31)$$

# Toy problem

## settings

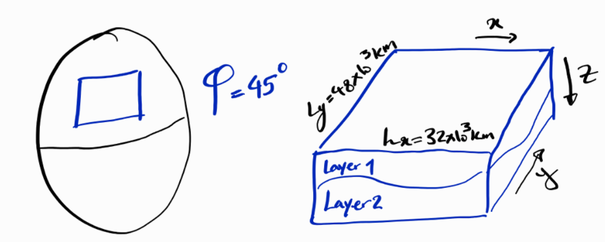


Figure: Schematic of the toy problem

$$\begin{aligned} L_x &= 32 \times 10^3\, km \rightarrow L_x^* \sim 46 \\ L_y &= 48 \times 10^3\, km \rightarrow L_y^* \sim 68 \end{aligned} \tag{32}$$

# Toy problem

settings

- Zonal direction ($X$): periodic boundary condition,
- Meridional direction ($Y$): Sponge boundary condition,
- Random initialization of the domain.

# Spectral Method

solution

## Governing Equations

$$\partial_t q_k + J(\psi_k, q_k) = -\frac{1}{\tau_d}(-1)^k(\psi_1 - \psi_2 - \psi_R) - \frac{1}{\tau_f}\delta_{k2}\nabla^2\psi_k - \nu\nabla^8 q_k$$
$$q_i = \nabla^2\psi_i + (-1)^k(\psi_1 - \psi_2) + \beta y \tag{33}$$

First we define

$$V_k = q_k - \beta y, \tag{34}$$

then we have

$$\partial_t q_k + J(\psi_k, V_k) + \beta\psi_x^k = -\frac{1}{\tau_d}(-1)^k(\psi_1 - \psi_2 - \psi_R) - \frac{1}{\tau_f}\delta_{k2}\nabla^2\psi_k - \nu\nabla^8 \tag{35}$$

# Spectral Method

solution

## Governing Equations

$$\partial_t q_k + J(\psi_k, V_k) + \beta\psi_x^k = -\frac{1}{\tau_d}(-1)^k(\psi_1 - \psi_2 - \psi_R) - \frac{1}{\tau_f}\delta_{k2}\nabla^2\psi_k - \nu\nabla^8$$
$$q_i = \nabla^2\psi_i + (-1)^k(\psi_1 - \psi_2) + \beta y \tag{36}$$

We take Fourier transform from these equations:

$$\begin{aligned}\frac{\partial F[q_k]}{\partial t} + F[J(\psi_k, V_k)] + \beta(-ik_x)F[\psi_k] &= -\frac{1}{\tau_d}(-1)^k(F[\psi_1] - F[\psi_2] - F[\psi_R]) \\ &+\frac{1}{\tau_f}\delta_{k2}(k_x^2 + k_y^2)F[\psi_k] - \nu(k_x^8 + k_y^8)F[q_k]\end{aligned} \tag{37}$$

$$F[V_k] = -(k_x^2 + k_y^2)F[\psi_k] + (-1)^k(F[\psi_1] - F[\psi_2]) \tag{38}$$

# Spectral Method

solution

## Governing Equations

$$
\begin{aligned}
\frac{\partial F[q_k]}{\partial t} + F[J(\psi_k, V_k)] + \beta(-ik_x)F[\psi_k] = -\frac{1}{\tau_d}(-1)^k(F[\psi_1] - F[\psi_2] - F[\psi_R]) \\
+\frac{1}{\tau_f}\delta_{k2}(k_x^2 + k_y^2)F[\psi_k] - \nu(k_x^8 + k_y^8)F[q_k]
\end{aligned}
$$

We have ODE for $F[q_k]$ as

$$
\begin{aligned}
\frac{\partial F[q_k]}{\partial t} &= RHS_k \\
RHS_k &= NN_k + Forces_k + Sponge_k + HD_K
\end{aligned} \tag{39}
$$

# Spectral Method

solution

We use Leapfrog + filtering to solve this ODE as:

- First time step (Euler-Backward):

$$F[q^n] = \frac{\Delta t}{1 + \Delta t \nu k^8} \left( \frac{F[q^{n-1}]}{\Delta t} + RHS_k \right) \tag{40}$$

- Other steps (Leapfrog):

$$F[q]_*^{n+1} = F[q]^{n-1} + 2\Delta t (F[q] + RHS)^{n+1} \tag{41}$$

$$F[q]^n = F[q]^n + g(F[q]^{n-1} - 2F[q]^n + F[q]_*^{n+1}) \tag{42}$$

- Then the second equation can be used to find $\psi_k$.
- $\Delta t^* = 0.025$ (non-dimensionalized) or $\Delta t \sim 7.3\, min$.

We want to solve following ODE,

$$\frac{dy}{dt} = f(t, y) + q_1(t) \qquad (43)$$
$$y(0) = y_0 + q_2$$

But we are not sure about: 1- our physical model and 2- initial condition.
In return we receive some observations in time.

$$g(y, t) + q_3(t) = 0 \qquad (44)$$

If there was no error in observations, we could

$$y_0^{num}, y_1^{num}, \ldots, y_{n-1}^{num}, y_n^{obs}, y_{n+1}^{num}, \ldots \qquad (45)$$

# Kalman Filter
## linear

For a linear state-space model:
Prediction:

$$\begin{aligned}\hat{x}_{k|k-1} &= A\hat{x}_{k-1|k-1} + Bu_k \\ P_{k|k-1} &= AP_{k-1|k-1}A^T + Q\end{aligned} \tag{46}$$

Update:

$$\begin{aligned}K_k &= P_{k|k-1}H^T(HP_{k|k-1}H^T + R)^{-1} \\ \hat{x}_{k|k} &= \hat{x}_{k|k-1} + K_k(z_k - H\hat{x}_{k|k-1}) \\ P_{k|k} &= (I - K_kH)P_{k|k-1}\end{aligned} \tag{47}$$

P: estimate covariance R: observation noise covariance

# Kalman Filter

non-linear

- Nonlinear state-space model,
- Linearizes around current estimate,

Prediction:

$$\begin{aligned} \hat{x}_{k|k-1} &= f(\hat{x}_{k-1|k-1}, u_k) \\ P_{k|k-1} &= F_{k-1} P_{k-1|k-1} F_{k-1}^T + Q \end{aligned} \tag{48}$$

Update:

$$\begin{aligned} K_k &= P_{k|k-1} H_k^T (H_k P_{k|k-1} H_k^T + R)^{-1} \\ \hat{x}_{k|k} &= \hat{x}_{k|k-1} + K_k (z_k - h(\hat{x}_{k|k-1})) \\ P_{k|k} &= (I - K_k H_k) P_{k|k-1} \end{aligned} \tag{49}$$

$F$: Jacobian of $f$ which is very expensive to calculate.

# Ensemble Kalman Filter

non-linear

- Nonlinear state-space model,
- Uses an ensemble of state vectors to estimate $P$,

$$\begin{aligned} \mathbf{x}_k^i &= f(\mathbf{x}_{k-1}^i) + \mathbf{w}_{k-1}^i \\ P_{k|k-1} &= \mathbb{E}\left[(\mathbf{X} - \bar{\mathbf{X}})(\mathbf{X} - \bar{\mathbf{X}})^T\right] \end{aligned} \tag{50}$$

Update:

$$\begin{aligned} \mathbf{K}_k &= P_{k|k-1}\left(P_{k|k-1} + R\right)^{-1} \\ \mathbf{x}_k^i &= \mathbf{x}_k^i + \mathbf{K}_k(\mathbf{z}_k^i - h(\mathbf{x}_k^i)) \end{aligned} \tag{51}$$

Forming $\mathbf{X}$ requires many simulations and is expensive for large number of variables.

# Hybrid Kalman Filter

## Machine learning

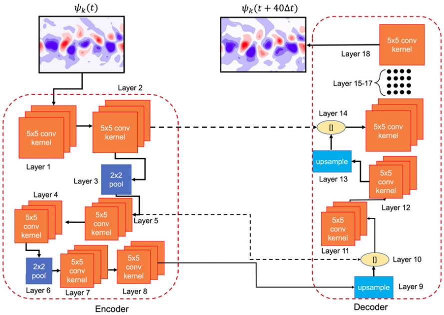


Figure: The U-NET model (surrogate) for approximating $\mathbf{X}$.

Source: Deep learning-enhanced ensemble-based data assimilation for high-dimensional nonlinear dynamical systems (2023).

# Hybrid Kalman Filter

## Machine learning

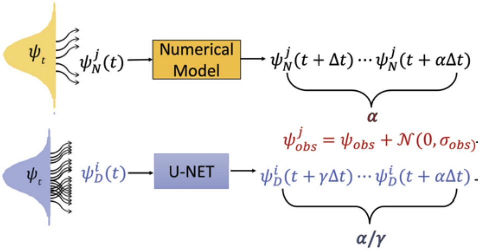


Figure: The U-NET model (surrogate) for approximating $\mathbf{X}$.

Source: Deep learning-enhanced ensemble-based data assimilation for high-dimensional nonlinear dynamical systems (2023).

# Hybrid Kalman Filter

## Machine learning

1. Solve numerically for one day,
   - $\Delta t \sim 7.3m$, about 200 iterations is necessary to simulate one physical day,
   - Ensemble of size 20 (different simulations at same time),
2. Use Kalman filter to update the state of the system $(192x96x2)$,
   - Generate 2000 different variations of the initial state variables,
   - Advance them using the surrogate model for one day,
   - Approximate $K$,
3. return to step 1